



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 9COJ
BMRB ID : 50957
Title : SH3-like tandem domain of human KIN protein
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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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.37.1

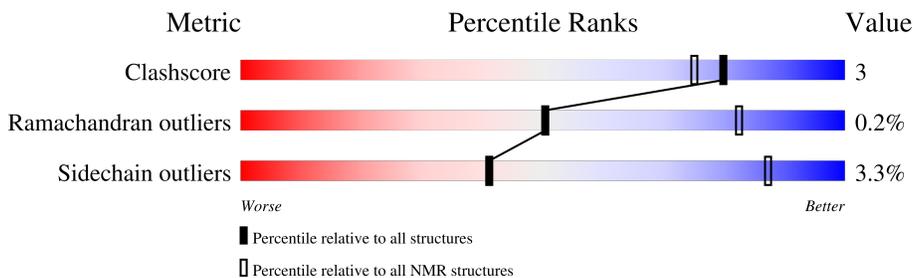
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

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 | 127 | |

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:13-A:127 (115) | 0.48 | 8 |

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2082 atoms, of which 1073 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA/RNA-binding protein KIN17.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 127 | 2082 | 643 | 1073 | 174 | 191 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

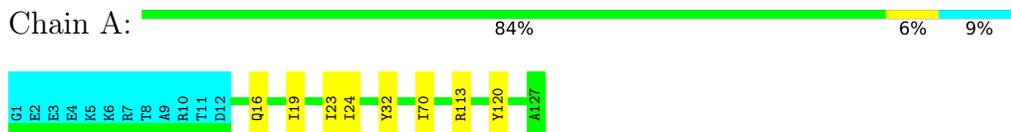
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1 | GLY | - | expression tag | UNP O60870 |

4 Residue-property plots [i](#)

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: DNA/RNA-binding protein KIN17

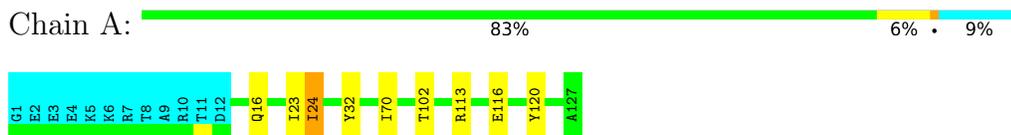


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

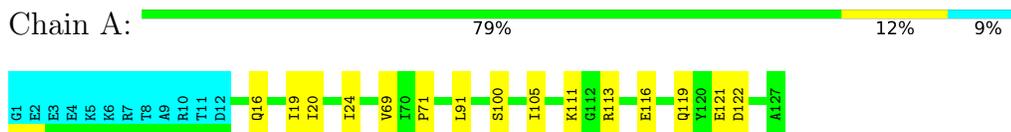
4.2.1 Score per residue for model 1

- Molecule 1: DNA/RNA-binding protein KIN17



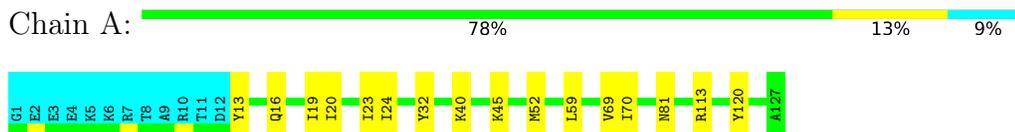
4.2.2 Score per residue for model 2

- Molecule 1: DNA/RNA-binding protein KIN17



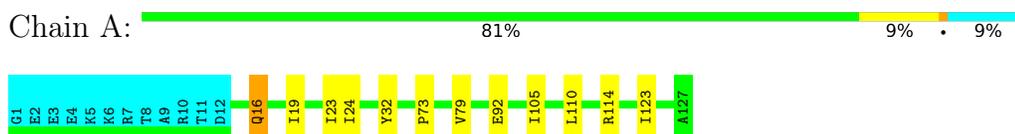
4.2.3 Score per residue for model 3

- Molecule 1: DNA/RNA-binding protein KIN17



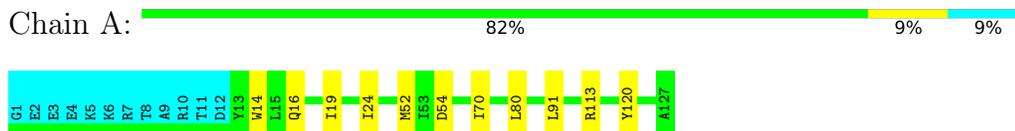
4.2.4 Score per residue for model 4

- Molecule 1: DNA/RNA-binding protein KIN17



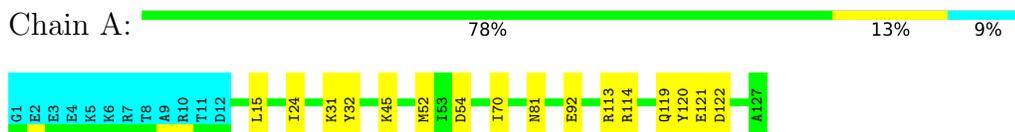
4.2.5 Score per residue for model 5

- Molecule 1: DNA/RNA-binding protein KIN17



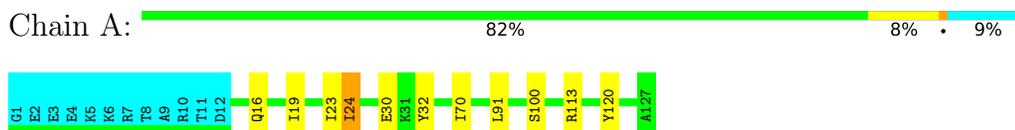
4.2.6 Score per residue for model 6

- Molecule 1: DNA/RNA-binding protein KIN17



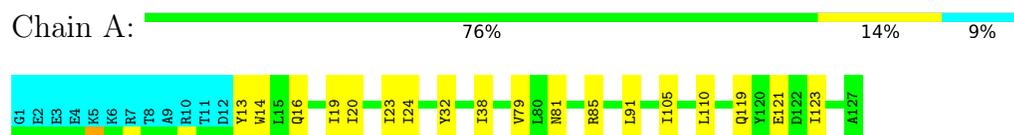
4.2.7 Score per residue for model 7

- Molecule 1: DNA/RNA-binding protein KIN17



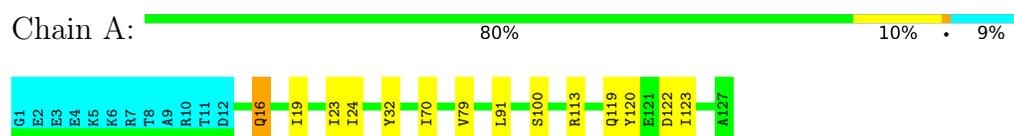
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: DNA/RNA-binding protein KIN17



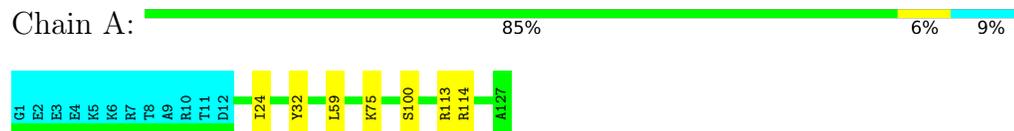
4.2.9 Score per residue for model 9

- Molecule 1: DNA/RNA-binding protein KIN17



4.2.10 Score per residue for model 10

- Molecule 1: DNA/RNA-binding protein KIN17



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| ARIA | refinement | 2.3.2 |
| CNS | structure calculation | |
| CNS | refinement | |
| ARIA | refinement | 2.3.2 |

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 | 1668 |
| Number of shifts mapped to atoms | 1668 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 94% |

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 911 | 975 | 973 | 5±2 |
| All | All | 9110 | 9750 | 9730 | 51 |

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 3.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:119:GLN:HB3 | 1:A:121:GLU:OE2 | 0.57 | 1.99 | 8 | 2 |
| 1:A:119:GLN:HB3 | 1:A:121:GLU:OE1 | 0.53 | 2.03 | 2 | 1 |
| 1:A:23:ILE:HB | 1:A:32:TYR:O | 0.52 | 2.04 | 4 | 6 |
| 1:A:119:GLN:HB2 | 1:A:122:ASP:OD2 | 0.52 | 2.05 | 6 | 2 |
| 1:A:16:GLN:O | 1:A:19:ILE:HG12 | 0.51 | 2.05 | 3 | 7 |
| 1:A:102:THR:HG23 | 1:A:116:GLU:HG2 | 0.50 | 1.82 | 1 | 1 |
| 1:A:13:TYR:OH | 1:A:85:ARG:HD2 | 0.50 | 2.06 | 8 | 1 |
| 1:A:119:GLN:HB2 | 1:A:122:ASP:OD1 | 0.49 | 2.07 | 2 | 1 |
| 1:A:70:ILE:HG13 | 1:A:120:TYR:CD2 | 0.49 | 2.43 | 9 | 4 |
| 1:A:31:LYS:HE2 | 1:A:32:TYR:CE1 | 0.48 | 2.42 | 6 | 1 |
| 1:A:70:ILE:HG13 | 1:A:120:TYR:CD1 | 0.48 | 2.44 | 6 | 2 |
| 1:A:52:MET:SD | 1:A:54:ASP:HB3 | 0.47 | 2.49 | 5 | 2 |
| 1:A:32:TYR:CD1 | 1:A:59:LEU:HD11 | 0.46 | 2.46 | 3 | 2 |
| 1:A:24:ILE:H | 1:A:24:ILE:HD13 | 0.46 | 1.70 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:105:ILE:HB | 1:A:110:LEU:O | 0.45 | 2.11 | 8 | 2 |
| 1:A:40:LYS:HE2 | 1:A:40:LYS:HA | 0.44 | 1.89 | 3 | 1 |
| 1:A:13:TYR:CB | 1:A:45:LYS:HB3 | 0.44 | 2.43 | 3 | 1 |
| 1:A:79:VAL:HA | 1:A:123:ILE:HG22 | 0.43 | 1.90 | 4 | 3 |
| 1:A:20:ILE:O | 1:A:69:VAL:HG22 | 0.43 | 2.14 | 3 | 2 |
| 1:A:73:PRO:HB3 | 1:A:92:GLU:O | 0.42 | 2.15 | 4 | 1 |
| 1:A:105:ILE:O | 1:A:111:LYS:HA | 0.41 | 2.14 | 2 | 1 |
| 1:A:92:GLU:OE2 | 1:A:114:ARG:HD2 | 0.41 | 2.15 | 6 | 1 |
| 1:A:20:ILE:CD1 | 1:A:38:ILE:HG12 | 0.41 | 2.45 | 8 | 1 |
| 1:A:32:TYR:CD1 | 1:A:52:MET:SD | 0.41 | 3.14 | 3 | 1 |
| 1:A:15:LEU:HB2 | 1:A:45:LYS:O | 0.41 | 2.16 | 6 | 1 |
| 1:A:92:GLU:OE1 | 1:A:114:ARG:HD2 | 0.40 | 2.15 | 4 | 1 |
| 1:A:14:TRP:O | 1:A:80:LEU:HB3 | 0.40 | 2.16 | 5 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|---------------|------------|------------|-------------|
| 1 | A | 114/127 (90%) | 108±2 (95±2%) | 6±2 (5±1%) | 0±0 (0±0%) | 50 82 |
| All | All | 1140/1270 (90%) | 1078 (95%) | 60 (5%) | 2 (0%) | 50 82 |

All 2 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 | 71 | PRO | 1 |
| 1 | A | 14 | TRP | 1 |

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|--------------|------------|-------------|
| 1 | A | 100/110 (91%) | 97±1 (97±1%) | 3±1 (3±1%) | 41 87 |
| All | All | 1000/1100 (91%) | 967 (97%) | 33 (3%) | 41 87 |

All 8 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 24 | ILE | 10 |
| 1 | A | 113 | ARG | 8 |
| 1 | A | 91 | LEU | 5 |
| 1 | A | 100 | SER | 4 |
| 1 | A | 16 | GLN | 3 |
| 1 | A | 30 | GLU | 1 |
| 1 | A | 75 | LYS | 1 |
| 1 | A | 114 | ARG | 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 monosaccharides 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 [i](#)

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping [i](#)

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

| | |
|---|------|
| Total number of shifts | 1668 |
| Number of shifts mapped to atoms | 1668 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 1 |

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 126 | -0.04 ± 0.17 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 116 | -0.04 ± 0.30 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 120 | 0.13 ± 0.12 | None needed (< 0.5 ppm) |
| ^{15}N | 120 | 1.43 ± 0.45 | Should be applied |

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1536 atoms were assigned a chemical shift out of a possible 1636. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 569/577 (99%) | 235/236 (100%) | 224/230 (97%) | 110/111 (99%) |
| Sidechain | 897/976 (92%) | 610/635 (96%) | 281/307 (92%) | 6/34 (18%) |

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| | Total | ¹H | ¹³C | ¹⁵N |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 70/83 (84%) | 35/39 (90%) | 34/39 (87%) | 1/5 (20%) |
| Overall | 1536/1636 (94%) | 880/910 (97%) | 539/576 (94%) | 117/150 (78%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1668 atoms were assigned a chemical shift out of a possible 1800. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone | 622/638 (97%) | 256/261 (98%) | 246/254 (97%) | 120/123 (98%) |
| Sidechain | 976/1079 (90%) | 663/698 (95%) | 307/339 (91%) | 6/42 (14%) |
| Aromatic | 70/83 (84%) | 35/39 (90%) | 34/39 (87%) | 1/5 (20%) |
| Overall | 1668/1800 (93%) | 954/998 (96%) | 587/632 (93%) | 127/170 (75%) |

7.1.4 Statistically unusual chemical shifts [i](#)

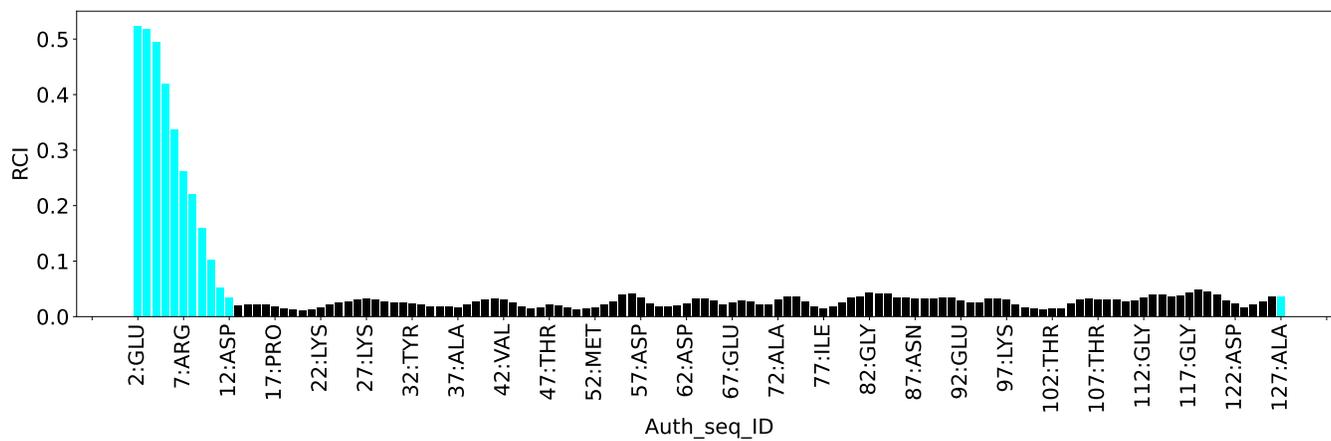
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 45 | LYS | HB3 | 0.34 | 0.46 – 3.04 | -5.5 |

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 5751 |
| Intra-residue ($ i-j =0$) | 2161 |
| Sequential ($ i-j =1$) | 1169 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 595 |
| Long range ($ i-j \geq 5$) | 1826 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 45.3 |
| Number of long range restraints per residue ¹ | 14.4 |

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) | 146.5 | 0.2 |
| 0.2-0.5 (Medium) | 257.8 | 0.5 |
| >0.5 (Large) | 203.5 | 3.7 |

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

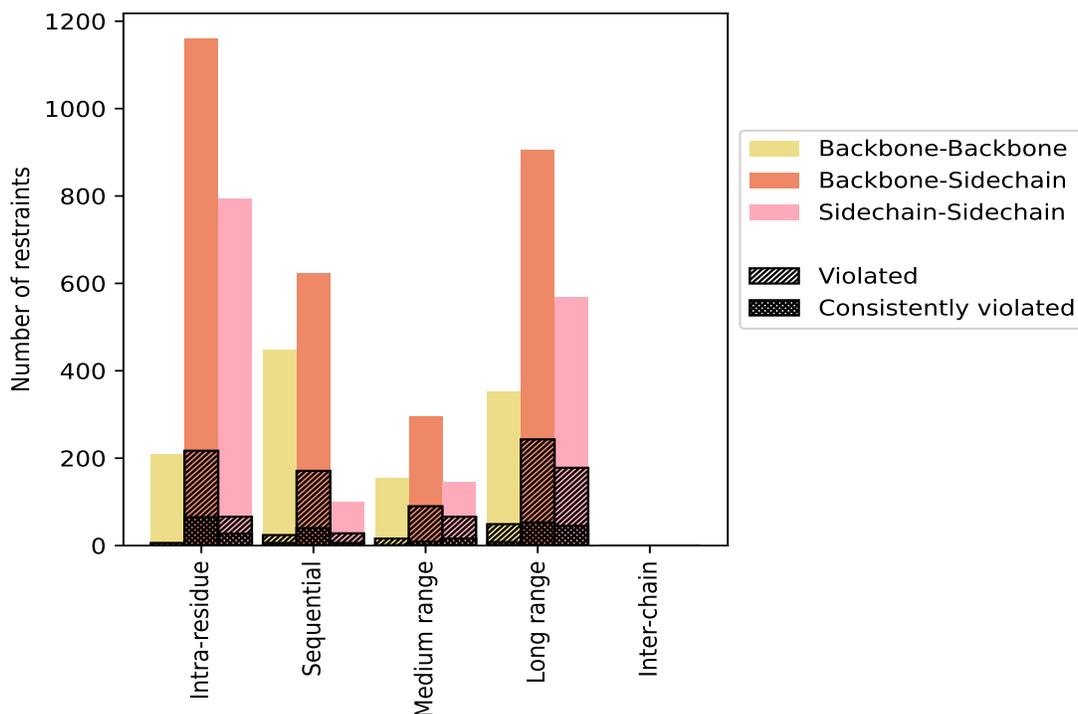
9.1 Summary of distance violations

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 2161 | 37.6 | 289 | 13.4 | 5.0 | 93 | 4.3 | 1.6 |
| Backbone-Backbone | 208 | 3.6 | 6 | 2.9 | 0.1 | 1 | 0.5 | 0.0 |
| Backbone-Sidechain | 1160 | 20.2 | 217 | 18.7 | 3.8 | 65 | 5.6 | 1.1 |
| Sidechain-Sidechain | 793 | 13.8 | 66 | 8.3 | 1.1 | 27 | 3.4 | 0.5 |
| Sequential ($i-j =1$) | 1169 | 20.3 | 223 | 19.1 | 3.9 | 52 | 4.4 | 0.9 |
| Backbone-Backbone | 447 | 7.8 | 24 | 5.4 | 0.4 | 6 | 1.3 | 0.1 |
| Backbone-Sidechain | 622 | 10.8 | 171 | 27.5 | 3.0 | 40 | 6.4 | 0.7 |
| Sidechain-Sidechain | 100 | 1.7 | 28 | 28.0 | 0.5 | 6 | 6.0 | 0.1 |
| Medium range ($i-j >1$ & $i-j <5$) | 595 | 10.3 | 172 | 28.9 | 3.0 | 26 | 4.4 | 0.5 |
| Backbone-Backbone | 154 | 2.7 | 16 | 10.4 | 0.3 | 1 | 0.6 | 0.0 |
| Backbone-Sidechain | 295 | 5.1 | 90 | 30.5 | 1.6 | 9 | 3.1 | 0.2 |
| Sidechain-Sidechain | 146 | 2.5 | 66 | 45.2 | 1.1 | 16 | 11.0 | 0.3 |
| Long range ($i-j \geq 5$) | 1826 | 31.8 | 470 | 25.7 | 8.2 | 106 | 5.8 | 1.8 |
| Backbone-Backbone | 351 | 6.1 | 49 | 14.0 | 0.9 | 8 | 2.3 | 0.1 |
| Backbone-Sidechain | 906 | 15.8 | 243 | 26.8 | 4.2 | 53 | 5.8 | 0.9 |
| Sidechain-Sidechain | 569 | 9.9 | 178 | 31.3 | 3.1 | 45 | 7.9 | 0.8 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 5751 | 100.0 | 1154 | 20.1 | 20.1 | 277 | 4.8 | 4.8 |
| Backbone-Backbone | 1160 | 20.2 | 95 | 8.2 | 1.7 | 16 | 1.4 | 0.3 |
| Backbone-Sidechain | 2983 | 51.9 | 721 | 24.2 | 12.5 | 167 | 5.6 | 2.9 |
| Sidechain-Sidechain | 1608 | 28.0 | 338 | 21.0 | 5.9 | 94 | 5.8 | 1.6 |

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 disulfid bonds are counted in their appropriate category on the x-axis

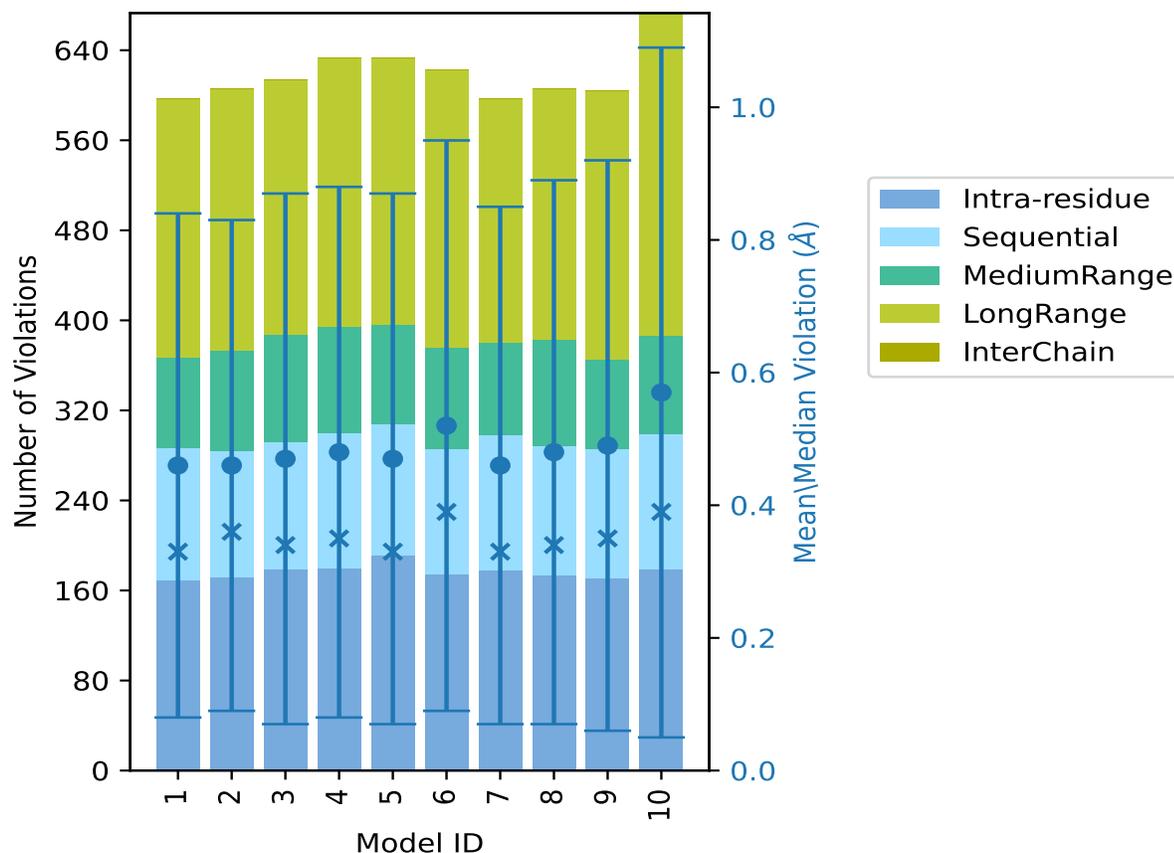
9.2 Distance violation statistics for each model [i](#)

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 | 169 | 118 | 80 | 230 | 0 | 597 | 0.46 | 2.43 | 0.38 | 0.33 |
| 2 | 172 | 112 | 89 | 233 | 0 | 606 | 0.46 | 2.83 | 0.37 | 0.36 |
| 3 | 179 | 113 | 95 | 227 | 0 | 614 | 0.47 | 2.88 | 0.4 | 0.34 |
| 4 | 180 | 120 | 94 | 239 | 0 | 633 | 0.48 | 2.69 | 0.4 | 0.35 |
| 5 | 191 | 117 | 88 | 237 | 0 | 633 | 0.47 | 2.97 | 0.4 | 0.33 |
| 6 | 174 | 112 | 90 | 247 | 0 | 623 | 0.52 | 3.24 | 0.43 | 0.39 |
| 7 | 178 | 120 | 82 | 217 | 0 | 597 | 0.46 | 2.52 | 0.39 | 0.33 |
| 8 | 174 | 114 | 95 | 223 | 0 | 606 | 0.48 | 2.65 | 0.41 | 0.34 |
| 9 | 171 | 115 | 79 | 239 | 0 | 604 | 0.49 | 2.72 | 0.43 | 0.35 |
| 10 | 179 | 120 | 87 | 287 | 0 | 673 | 0.57 | 3.7 | 0.52 | 0.39 |

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 [i](#)



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4597(IR:1872, SQ:946, MR:423, LR:1356, 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 | % |
| 52 | 46 | 29 | 120 | 0 | 247 | 1 | 10.0 |
| 33 | 33 | 23 | 51 | 0 | 140 | 2 | 20.0 |
| 16 | 17 | 13 | 37 | 0 | 83 | 3 | 30.0 |

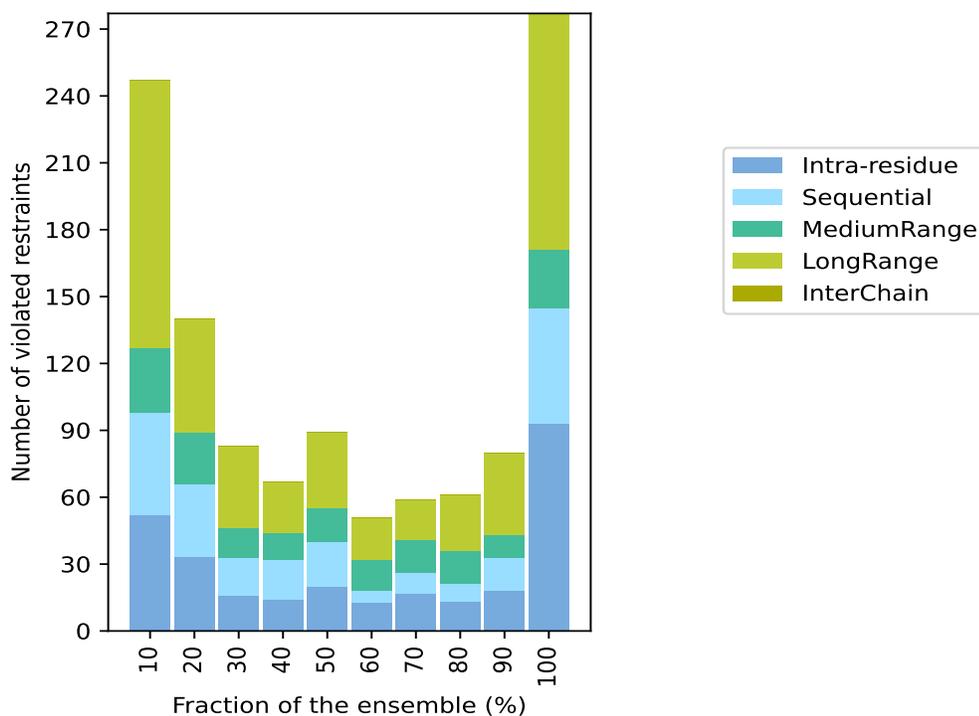
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 14 | 18 | 12 | 23 | 0 | 67 | 4 | 40.0 |
| 20 | 20 | 15 | 34 | 0 | 89 | 5 | 50.0 |
| 13 | 5 | 14 | 19 | 0 | 51 | 6 | 60.0 |
| 17 | 9 | 15 | 18 | 0 | 59 | 7 | 70.0 |
| 13 | 8 | 15 | 25 | 0 | 61 | 8 | 80.0 |
| 18 | 15 | 10 | 37 | 0 | 80 | 9 | 90.0 |
| 93 | 52 | 26 | 106 | 0 | 277 | 10 | 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](#)

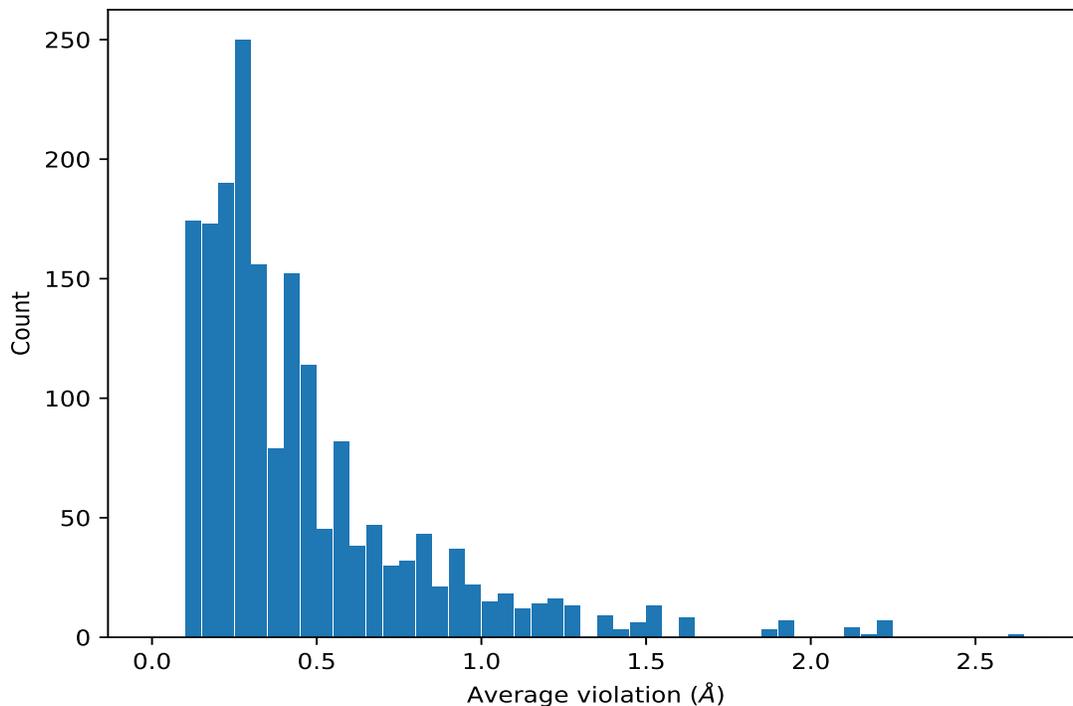


9.4 Most violated distance restraints in the ensemble [i](#)

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) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,250) | 1:15:A:LEU:HD11 | 1:66:A:LEU:HD22 | 10 | 2.2 | 0.08 | 2.19 |
| (3,250) | 1:15:A:LEU:HD12 | 1:66:A:LEU:HD21 | 10 | 2.2 | 0.08 | 2.19 |
| (3,250) | 1:15:A:LEU:HD11 | 1:66:A:LEU:HD23 | 10 | 2.2 | 0.08 | 2.19 |
| (3,250) | 1:15:A:LEU:HD12 | 1:66:A:LEU:HD23 | 10 | 2.2 | 0.08 | 2.19 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD23 | 10 | 2.2 | 0.08 | 2.19 |
| (3,250) | 1:15:A:LEU:HD12 | 1:66:A:LEU:HD22 | 10 | 2.2 | 0.08 | 2.19 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD21 | 10 | 2.2 | 0.08 | 2.19 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 10 | 2.15 | 0.17 | 2.12 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 10 | 2.13 | 0.31 | 2.22 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 10 | 2.13 | 0.31 | 2.22 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 10 | 2.13 | 0.31 | 2.22 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 10 | 2.1 | 0.23 | 2.16 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 10 | 1.93 | 0.73 | 2.06 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 10 | 1.93 | 0.73 | 2.06 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 10 | 1.93 | 0.73 | 2.06 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 10 | 1.64 | 0.82 | 1.6 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 10 | 1.64 | 0.82 | 1.6 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 10 | 1.64 | 0.82 | 1.6 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 10 | 1.61 | 0.09 | 1.62 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 10 | 1.61 | 0.09 | 1.62 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 10 | 1.61 | 0.09 | 1.62 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 10 | 1.53 | 0.16 | 1.5 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 10 | 1.53 | 0.16 | 1.5 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 10 | 1.53 | 0.16 | 1.5 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 10 | 1.52 | 0.77 | 1.53 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 10 | 1.5 | 0.12 | 1.51 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 10 | 1.48 | 0.11 | 1.46 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 10 | 1.48 | 0.08 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 10 | 1.48 | 0.08 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 10 | 1.48 | 0.08 | 1.5 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 10 | 1.48 | 0.2 | 1.46 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 10 | 1.44 | 0.19 | 1.46 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 10 | 1.43 | 0.2 | 1.42 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 10 | 1.39 | 0.25 | 1.39 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 10 | 1.29 | 0.08 | 1.32 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 10 | 1.26 | 0.16 | 1.25 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 10 | 1.26 | 0.16 | 1.18 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 10 | 1.25 | 0.05 | 1.27 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 10 | 1.23 | 0.15 | 1.18 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 10 | 1.22 | 0.16 | 1.18 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 10 | 1.22 | 0.16 | 1.18 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 10 | 1.22 | 0.16 | 1.18 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 10 | 1.16 | 0.2 | 1.14 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 10 | 1.16 | 0.2 | 1.14 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 10 | 1.16 | 0.2 | 1.14 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 10 | 1.14 | 0.07 | 1.14 |
| (3,927) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 10 | 1.1 | 0.01 | 1.1 |
| (3,927) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 10 | 1.1 | 0.01 | 1.1 |
| (3,927) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 10 | 1.1 | 0.01 | 1.1 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 10 | 1.09 | 0.15 | 1.13 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 10 | 1.08 | 0.48 | 0.89 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 10 | 1.08 | 0.37 | 1.15 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 10 | 1.07 | 0.11 | 1.05 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 10 | 1.02 | 0.13 | 1.05 |
| (3,501) | 1:49:A:VAL:HG11 | 1:40:A:LYS:HB3 | 10 | 1.02 | 0.23 | 1.04 |
| (3,501) | 1:49:A:VAL:HG13 | 1:40:A:LYS:HB3 | 10 | 1.02 | 0.23 | 1.04 |
| (3,501) | 1:49:A:VAL:HG12 | 1:40:A:LYS:HB3 | 10 | 1.02 | 0.23 | 1.04 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 10 | 1.01 | 0.01 | 1.01 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 10 | 1.01 | 0.03 | 1.0 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 10 | 1.0 | 0.21 | 0.98 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 10 | 0.98 | 0.16 | 0.96 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 10 | 0.97 | 0.23 | 1.02 |
| (3,814) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 10 | 0.96 | 0.22 | 0.96 |
| (3,814) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 10 | 0.96 | 0.22 | 0.96 |
| (3,814) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 10 | 0.96 | 0.22 | 0.96 |
| (3,389) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HG3 | 10 | 0.95 | 0.18 | 0.89 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD11 | 10 | 0.95 | 0.18 | 0.89 |
| (3,389) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HG3 | 10 | 0.95 | 0.18 | 0.89 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD12 | 10 | 0.95 | 0.18 | 0.89 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD13 | 10 | 0.95 | 0.18 | 0.89 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 10 | 0.94 | 0.92 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 10 | 0.94 | 0.92 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 10 | 0.94 | 0.92 | 0.67 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 10 | 0.94 | 0.08 | 0.96 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 10 | 0.94 | 0.08 | 0.96 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 10 | 0.94 | 0.08 | 0.96 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 10 | 0.93 | 0.11 | 0.9 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 10 | 0.93 | 0.11 | 0.9 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 10 | 0.93 | 0.11 | 0.9 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 10 | 0.92 | 0.13 | 0.9 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 10 | 0.9 | 0.24 | 0.87 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 10 | 0.9 | 0.01 | 0.9 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 10 | 0.9 | 0.53 | 0.7 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 10 | 0.9 | 0.53 | 0.7 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 10 | 0.9 | 0.53 | 0.7 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 10 | 0.87 | 0.31 | 0.86 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 10 | 0.87 | 0.09 | 0.84 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 10 | 0.86 | 0.13 | 0.85 |
| (3,892) | 1:25:A:THR:HG21 | 1:25:A:THR:HA | 10 | 0.86 | 0.03 | 0.87 |
| (3,892) | 1:25:A:THR:HG23 | 1:25:A:THR:HA | 10 | 0.86 | 0.03 | 0.87 |
| (3,892) | 1:25:A:THR:HG22 | 1:25:A:THR:HA | 10 | 0.86 | 0.03 | 0.87 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 10 | 0.86 | 0.02 | 0.85 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 10 | 0.84 | 0.22 | 0.8 |
| (3,735) | 1:115:A:VAL:HG13 | 1:103:A:ILE:HD12 | 10 | 0.83 | 0.59 | 0.8 |
| (3,735) | 1:115:A:VAL:HG11 | 1:103:A:ILE:HD13 | 10 | 0.83 | 0.59 | 0.8 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD11 | 10 | 0.83 | 0.59 | 0.8 |
| (3,735) | 1:115:A:VAL:HG13 | 1:103:A:ILE:HD11 | 10 | 0.83 | 0.59 | 0.8 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD13 | 10 | 0.83 | 0.59 | 0.8 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD12 | 10 | 0.83 | 0.59 | 0.8 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,735) | 1:115:A:VAL:HG13 | 1:103:A:ILE:HD13 | 10 | 0.83 | 0.59 | 0.8 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 10 | 0.83 | 0.04 | 0.86 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 10 | 0.82 | 0.24 | 0.74 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 10 | 0.82 | 0.52 | 0.68 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 10 | 0.82 | 0.52 | 0.68 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 10 | 0.82 | 0.52 | 0.68 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD11 | 10 | 0.81 | 0.22 | 0.82 |
| (3,401) | 1:15:A:LEU:HD22 | 1:80:A:LEU:HD13 | 10 | 0.81 | 0.22 | 0.82 |
| (3,401) | 1:15:A:LEU:HD22 | 1:80:A:LEU:HD11 | 10 | 0.81 | 0.22 | 0.82 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD13 | 10 | 0.81 | 0.22 | 0.82 |
| (3,401) | 1:15:A:LEU:HD21 | 1:80:A:LEU:HD12 | 10 | 0.81 | 0.22 | 0.82 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD12 | 10 | 0.81 | 0.22 | 0.82 |
| (3,401) | 1:15:A:LEU:HD23 | 1:66:A:LEU:HD23 | 10 | 0.81 | 0.22 | 0.82 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 10 | 0.8 | 0.22 | 0.88 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 10 | 0.8 | 0.22 | 0.88 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 10 | 0.8 | 0.22 | 0.88 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 10 | 0.79 | 0.15 | 0.78 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 10 | 0.79 | 0.1 | 0.82 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 10 | 0.78 | 0.07 | 0.75 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD13 | 10 | 0.78 | 0.15 | 0.8 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD11 | 10 | 0.78 | 0.15 | 0.8 |
| (3,603) | 1:25:A:THR:HG21 | 1:23:A:ILE:HD12 | 10 | 0.78 | 0.15 | 0.8 |
| (3,603) | 1:25:A:THR:HG23 | 1:23:A:ILE:HD13 | 10 | 0.78 | 0.15 | 0.8 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD12 | 10 | 0.78 | 0.15 | 0.8 |
| (3,603) | 1:25:A:THR:HG21 | 1:23:A:ILE:HD13 | 10 | 0.78 | 0.15 | 0.8 |
| (3,603) | 1:25:A:THR:HG23 | 1:23:A:ILE:HD11 | 10 | 0.78 | 0.15 | 0.8 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 10 | 0.75 | 0.23 | 0.68 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 10 | 0.75 | 0.23 | 0.68 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 10 | 0.75 | 0.23 | 0.68 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 10 | 0.75 | 0.41 | 0.78 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 10 | 0.75 | 0.41 | 0.78 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 10 | 0.75 | 0.41 | 0.78 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 10 | 0.74 | 0.0 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 10 | 0.74 | 0.0 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 10 | 0.74 | 0.0 | 0.74 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 10 | 0.74 | 0.21 | 0.73 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 10 | 0.74 | 0.09 | 0.73 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 10 | 0.74 | 0.09 | 0.73 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 10 | 0.74 | 0.09 | 0.73 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 10 | 0.73 | 0.12 | 0.78 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 10 | 0.73 | 0.11 | 0.7 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 10 | 0.73 | 0.11 | 0.7 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 10 | 0.73 | 0.11 | 0.7 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 10 | 0.73 | 0.19 | 0.73 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 10 | 0.72 | 0.1 | 0.69 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 10 | 0.72 | 0.1 | 0.69 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 10 | 0.72 | 0.1 | 0.69 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG23 | 10 | 0.72 | 0.1 | 0.74 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG22 | 10 | 0.72 | 0.1 | 0.74 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG21 | 10 | 0.72 | 0.1 | 0.74 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 10 | 0.71 | 0.14 | 0.7 |
| (3,850) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HH2 | 10 | 0.71 | 0.11 | 0.72 |
| (3,850) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HH2 | 10 | 0.71 | 0.11 | 0.72 |
| (3,850) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HH2 | 10 | 0.71 | 0.11 | 0.72 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG21 | 10 | 0.71 | 0.07 | 0.69 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG22 | 10 | 0.71 | 0.07 | 0.69 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG23 | 10 | 0.71 | 0.07 | 0.69 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 10 | 0.7 | 0.11 | 0.72 |
| (3,795) | 1:52:A:MET:H | 1:56:A:GLY:HA3 | 10 | 0.7 | 0.11 | 0.72 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 10 | 0.69 | 0.13 | 0.7 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG22 | 10 | 0.69 | 0.13 | 0.7 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG21 | 10 | 0.69 | 0.13 | 0.7 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB2 | 10 | 0.69 | 0.12 | 0.7 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB3 | 10 | 0.69 | 0.12 | 0.7 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB1 | 10 | 0.69 | 0.12 | 0.7 |
| (3,162) | 1:15:A:LEU:H | 1:19:A:ILE:HD11 | 10 | 0.69 | 0.12 | 0.7 |
| (3,162) | 1:15:A:LEU:H | 1:19:A:ILE:HD13 | 10 | 0.69 | 0.12 | 0.7 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 10 | 0.68 | 0.22 | 0.64 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 10 | 0.67 | 0.22 | 0.68 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 10 | 0.67 | 0.22 | 0.68 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 10 | 0.67 | 0.22 | 0.68 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 10 | 0.67 | 0.2 | 0.68 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 10 | 0.67 | 0.2 | 0.68 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 10 | 0.67 | 0.04 | 0.67 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 10 | 0.67 | 0.03 | 0.66 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 10 | 0.66 | 0.2 | 0.62 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 10 | 0.66 | 0.2 | 0.62 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 10 | 0.66 | 0.2 | 0.62 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 10 | 0.65 | 0.21 | 0.71 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 10 | 0.64 | 0.04 | 0.66 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 10 | 0.64 | 0.21 | 0.58 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 10 | 0.64 | 0.28 | 0.78 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 10 | 0.64 | 0.28 | 0.78 |
| (3,1036) | 1:21:A:VAL:HG13 | 1:22:A:LYS:H | 10 | 0.62 | 0.05 | 0.63 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,1036) | 1:21:A:VAL:HG12 | 1:22:A:LYS:H | 10 | 0.62 | 0.05 | 0.63 |
| (3,1036) | 1:21:A:VAL:HG11 | 1:22:A:LYS:H | 10 | 0.62 | 0.05 | 0.63 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 10 | 0.61 | 0.23 | 0.54 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 10 | 0.61 | 0.23 | 0.54 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 10 | 0.61 | 0.23 | 0.54 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 10 | 0.61 | 0.05 | 0.6 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 10 | 0.61 | 0.03 | 0.61 |
| (3,995) | 1:79:A:VAL:HG22 | 1:79:A:VAL:H | 10 | 0.61 | 0.19 | 0.68 |
| (3,995) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 10 | 0.61 | 0.19 | 0.68 |
| (3,995) | 1:102:A:THR:HG23 | 1:116:A:GLU:H | 10 | 0.61 | 0.19 | 0.68 |
| (3,995) | 1:102:A:THR:HG22 | 1:116:A:GLU:H | 10 | 0.61 | 0.19 | 0.68 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 10 | 0.6 | 0.24 | 0.6 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 10 | 0.6 | 0.38 | 0.54 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 10 | 0.6 | 0.38 | 0.54 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 10 | 0.59 | 0.03 | 0.6 |
| (3,449) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 10 | 0.58 | 0.01 | 0.58 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG22 | 10 | 0.58 | 0.01 | 0.58 |
| (3,449) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG23 | 10 | 0.58 | 0.01 | 0.58 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG23 | 10 | 0.58 | 0.01 | 0.58 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG21 | 10 | 0.58 | 0.01 | 0.58 |
| (3,449) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG22 | 10 | 0.58 | 0.01 | 0.58 |
| (3,449) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG23 | 10 | 0.58 | 0.01 | 0.58 |
| (3,399) | 1:43:A:ILE:HG22 | 1:44:A:ASP:HA | 10 | 0.58 | 0.22 | 0.64 |
| (3,399) | 1:45:A:LYS:HG3 | 1:44:A:ASP:HA | 10 | 0.58 | 0.22 | 0.64 |
| (3,399) | 1:43:A:ILE:HG21 | 1:44:A:ASP:HA | 10 | 0.58 | 0.22 | 0.64 |
| (3,399) | 1:43:A:ILE:HG23 | 1:44:A:ASP:HA | 10 | 0.58 | 0.22 | 0.64 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 10 | 0.58 | 0.09 | 0.58 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 10 | 0.58 | 0.09 | 0.58 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 10 | 0.57 | 0.02 | 0.56 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 10 | 0.56 | 0.17 | 0.52 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 10 | 0.55 | 0.01 | 0.56 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 10 | 0.55 | 0.01 | 0.56 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 10 | 0.55 | 0.01 | 0.56 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 10 | 0.54 | 0.01 | 0.55 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 10 | 0.54 | 0.01 | 0.55 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 10 | 0.54 | 0.01 | 0.55 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 10 | 0.53 | 0.04 | 0.54 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 10 | 0.53 | 0.01 | 0.54 |
| (3,1155) | 1:118:A:ILE:HG23 | 1:119:A:GLN:H | 10 | 0.52 | 0.12 | 0.55 |
| (3,1155) | 1:118:A:ILE:HG21 | 1:119:A:GLN:H | 10 | 0.52 | 0.12 | 0.55 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 10 | 0.52 | 0.12 | 0.55 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 10 | 0.51 | 0.01 | 0.52 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 10 | 0.51 | 0.01 | 0.52 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 10 | 0.51 | 0.01 | 0.52 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 10 | 0.49 | 0.08 | 0.52 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 10 | 0.49 | 0.12 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 10 | 0.49 | 0.11 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 10 | 0.49 | 0.11 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 10 | 0.49 | 0.11 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 10 | 0.49 | 0.11 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 10 | 0.49 | 0.11 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 10 | 0.49 | 0.11 | 0.52 |
| (3,879) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HB | 10 | 0.48 | 0.01 | 0.48 |
| (3,879) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HB | 10 | 0.48 | 0.01 | 0.48 |
| (3,879) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HB | 10 | 0.48 | 0.01 | 0.48 |
| (3,879) | 1:49:A:VAL:HB | 1:49:A:VAL:HG23 | 10 | 0.48 | 0.01 | 0.48 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 10 | 0.48 | 0.09 | 0.5 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 10 | 0.48 | 0.09 | 0.5 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 10 | 0.48 | 0.09 | 0.5 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 10 | 0.48 | 0.0 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 10 | 0.48 | 0.0 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 10 | 0.48 | 0.0 | 0.48 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD11 | 10 | 0.48 | 0.09 | 0.48 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 10 | 0.48 | 0.09 | 0.48 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD12 | 10 | 0.48 | 0.09 | 0.48 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 10 | 0.48 | 0.17 | 0.51 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 10 | 0.48 | 0.17 | 0.51 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 10 | 0.48 | 0.17 | 0.51 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 10 | 0.47 | 0.13 | 0.44 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 10 | 0.47 | 0.11 | 0.44 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 10 | 0.47 | 0.07 | 0.45 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 10 | 0.47 | 0.02 | 0.46 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 10 | 0.46 | 0.22 | 0.44 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 10 | 0.46 | 0.22 | 0.44 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 10 | 0.46 | 0.22 | 0.44 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 10 | 0.46 | 0.08 | 0.49 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 10 | 0.46 | 0.08 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 10 | 0.46 | 0.08 | 0.49 |
| (3,1093) | 1:70:A:ILE:HD13 | 1:123:A:ILE:H | 10 | 0.46 | 0.07 | 0.45 |
| (3,1093) | 1:70:A:ILE:HD11 | 1:123:A:ILE:H | 10 | 0.46 | 0.07 | 0.45 |
| (3,1093) | 1:70:A:ILE:HD12 | 1:123:A:ILE:H | 10 | 0.46 | 0.07 | 0.45 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 10 | 0.45 | 0.1 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 10 | 0.45 | 0.1 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 10 | 0.45 | 0.1 | 0.44 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 10 | 0.45 | 0.1 | 0.44 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 10 | 0.45 | 0.0 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 10 | 0.45 | 0.0 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 10 | 0.45 | 0.0 | 0.45 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD13 | 10 | 0.45 | 0.16 | 0.41 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD12 | 10 | 0.45 | 0.16 | 0.41 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD11 | 10 | 0.45 | 0.16 | 0.41 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 10 | 0.45 | 0.03 | 0.44 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 10 | 0.44 | 0.13 | 0.42 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 10 | 0.44 | 0.13 | 0.42 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 10 | 0.44 | 0.13 | 0.42 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 10 | 0.44 | 0.15 | 0.38 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 10 | 0.44 | 0.15 | 0.38 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 10 | 0.44 | 0.15 | 0.38 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 10 | 0.44 | 0.08 | 0.46 |
| (3,568) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HD23 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:19:A:ILE:HG21 | 1:78:A:LEU:HD11 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HD21 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:19:A:ILE:HG21 | 1:78:A:LEU:HD13 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:19:A:ILE:HG22 | 1:78:A:LEU:HD12 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:78:A:LEU:HD13 | 1:78:A:LEU:HD22 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:78:A:LEU:HD12 | 1:78:A:LEU:HD22 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HD22 | 10 | 0.44 | 0.05 | 0.46 |
| (3,568) | 1:19:A:ILE:HG23 | 1:78:A:LEU:HD12 | 10 | 0.44 | 0.05 | 0.46 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 10 | 0.44 | 0.09 | 0.45 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 10 | 0.44 | 0.09 | 0.45 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 10 | 0.44 | 0.09 | 0.45 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 10 | 0.44 | 0.08 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 10 | 0.43 | 0.03 | 0.43 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 10 | 0.43 | 0.03 | 0.43 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 10 | 0.43 | 0.09 | 0.44 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 10 | 0.43 | 0.09 | 0.44 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 10 | 0.43 | 0.09 | 0.44 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 10 | 0.43 | 0.1 | 0.44 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 10 | 0.43 | 0.1 | 0.44 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 10 | 0.43 | 0.1 | 0.44 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 10 | 0.43 | 0.0 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 10 | 0.43 | 0.0 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 10 | 0.43 | 0.0 | 0.43 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 10 | 0.43 | 0.07 | 0.42 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 10 | 0.43 | 0.08 | 0.44 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 10 | 0.43 | 0.08 | 0.44 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD12 | 10 | 0.42 | 0.01 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD13 | 10 | 0.42 | 0.01 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD11 | 10 | 0.42 | 0.01 | 0.42 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 10 | 0.42 | 0.02 | 0.42 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 10 | 0.42 | 0.07 | 0.42 |
| (3,371) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 10 | 0.42 | 0.07 | 0.42 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG22 | 10 | 0.42 | 0.08 | 0.42 |
| (3,841) | 1:80:A:LEU:HD21 | 1:80:A:LEU:H | 10 | 0.42 | 0.08 | 0.42 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG23 | 10 | 0.42 | 0.08 | 0.42 |
| (3,841) | 1:80:A:LEU:HD22 | 1:80:A:LEU:H | 10 | 0.42 | 0.08 | 0.42 |
| (3,841) | 1:80:A:LEU:HD23 | 1:80:A:LEU:H | 10 | 0.42 | 0.08 | 0.42 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 10 | 0.41 | 0.12 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 10 | 0.41 | 0.12 | 0.41 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 10 | 0.41 | 0.12 | 0.41 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 10 | 0.41 | 0.05 | 0.43 |
| (3,471) | 1:127:A:ALA:HB1 | 1:20:A:ILE:H | 10 | 0.41 | 0.05 | 0.43 |
| (3,471) | 1:127:A:ALA:HB3 | 1:20:A:ILE:H | 10 | 0.41 | 0.05 | 0.43 |
| (3,471) | 1:127:A:ALA:HB2 | 1:20:A:ILE:H | 10 | 0.41 | 0.05 | 0.43 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 10 | 0.41 | 0.07 | 0.42 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 10 | 0.41 | 0.08 | 0.42 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HG2 | 10 | 0.41 | 0.22 | 0.34 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HG2 | 10 | 0.41 | 0.22 | 0.34 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:110:A:LEU:HB2 | 10 | 0.41 | 0.22 | 0.34 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:110:A:LEU:HB2 | 10 | 0.41 | 0.22 | 0.34 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 10 | 0.41 | 0.14 | 0.41 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 10 | 0.41 | 0.14 | 0.41 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 10 | 0.41 | 0.14 | 0.41 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 10 | 0.41 | 0.08 | 0.41 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 10 | 0.41 | 0.08 | 0.41 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 10 | 0.41 | 0.08 | 0.41 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 10 | 0.41 | 0.08 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 10 | 0.4 | 0.01 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 10 | 0.4 | 0.0 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 10 | 0.4 | 0.0 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 10 | 0.4 | 0.0 | 0.4 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG23 | 10 | 0.4 | 0.06 | 0.4 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG21 | 10 | 0.4 | 0.06 | 0.4 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG22 | 10 | 0.4 | 0.06 | 0.4 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 10 | 0.4 | 0.16 | 0.4 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 10 | 0.4 | 0.16 | 0.4 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 10 | 0.4 | 0.16 | 0.4 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 10 | 0.4 | 0.09 | 0.4 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 10 | 0.4 | 0.05 | 0.4 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 10 | 0.39 | 0.1 | 0.42 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 10 | 0.39 | 0.1 | 0.37 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 10 | 0.39 | 0.05 | 0.39 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 10 | 0.39 | 0.07 | 0.38 |
| (3,600) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 10 | 0.39 | 0.07 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 10 | 0.38 | 0.12 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 10 | 0.38 | 0.12 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 10 | 0.38 | 0.12 | 0.38 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 10 | 0.38 | 0.13 | 0.42 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 10 | 0.38 | 0.13 | 0.42 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 10 | 0.38 | 0.13 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 10 | 0.38 | 0.08 | 0.4 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 10 | 0.38 | 0.08 | 0.4 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 10 | 0.38 | 0.08 | 0.4 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 10 | 0.38 | 0.04 | 0.38 |
| (3,1178) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HG2 | 10 | 0.38 | 0.04 | 0.38 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 10 | 0.38 | 0.04 | 0.39 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 10 | 0.38 | 0.04 | 0.39 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 10 | 0.38 | 0.04 | 0.39 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 10 | 0.37 | 0.04 | 0.38 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 10 | 0.36 | 0.08 | 0.37 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 10 | 0.36 | 0.08 | 0.37 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 10 | 0.36 | 0.08 | 0.37 |
| (3,751) | 1:43:A:ILE:HG22 | 1:43:A:ILE:H | 10 | 0.36 | 0.05 | 0.36 |
| (3,751) | 1:43:A:ILE:HG21 | 1:43:A:ILE:H | 10 | 0.36 | 0.05 | 0.36 |
| (3,751) | 1:43:A:ILE:HG23 | 1:43:A:ILE:H | 10 | 0.36 | 0.05 | 0.36 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG23 | 10 | 0.35 | 0.07 | 0.36 |
| (3,951) | 1:80:A:LEU:HD13 | 1:124:A:SER:H | 10 | 0.35 | 0.07 | 0.36 |
| (3,951) | 1:80:A:LEU:HD12 | 1:124:A:SER:H | 10 | 0.35 | 0.07 | 0.36 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG21 | 10 | 0.35 | 0.07 | 0.36 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG22 | 10 | 0.35 | 0.07 | 0.36 |
| (3,951) | 1:80:A:LEU:HD11 | 1:124:A:SER:H | 10 | 0.35 | 0.07 | 0.36 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 10 | 0.35 | 0.03 | 0.35 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 10 | 0.35 | 0.12 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 10 | 0.35 | 0.12 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 10 | 0.35 | 0.12 | 0.29 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 10 | 0.35 | 0.1 | 0.36 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 10 | 0.35 | 0.1 | 0.36 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 10 | 0.35 | 0.1 | 0.36 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 10 | 0.35 | 0.09 | 0.36 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 10 | 0.35 | 0.09 | 0.36 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 10 | 0.35 | 0.09 | 0.36 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 10 | 0.34 | 0.14 | 0.36 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 10 | 0.34 | 0.14 | 0.36 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 10 | 0.34 | 0.14 | 0.36 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 10 | 0.34 | 0.12 | 0.36 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 10 | 0.34 | 0.0 | 0.34 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 10 | 0.34 | 0.16 | 0.28 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 10 | 0.34 | 0.0 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 10 | 0.34 | 0.0 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 10 | 0.34 | 0.0 | 0.34 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 10 | 0.34 | 0.18 | 0.29 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 10 | 0.34 | 0.12 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 10 | 0.34 | 0.12 | 0.39 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 10 | 0.34 | 0.12 | 0.39 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 10 | 0.33 | 0.02 | 0.33 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 10 | 0.33 | 0.04 | 0.34 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 10 | 0.33 | 0.1 | 0.32 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 10 | 0.33 | 0.05 | 0.34 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 10 | 0.33 | 0.05 | 0.34 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 10 | 0.33 | 0.05 | 0.34 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 10 | 0.32 | 0.08 | 0.32 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 10 | 0.32 | 0.06 | 0.34 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 10 | 0.32 | 0.07 | 0.3 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 10 | 0.32 | 0.07 | 0.3 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 10 | 0.32 | 0.07 | 0.3 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 10 | 0.32 | 0.22 | 0.2 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 10 | 0.32 | 0.1 | 0.35 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 10 | 0.32 | 0.1 | 0.35 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 10 | 0.32 | 0.1 | 0.35 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 10 | 0.32 | 0.04 | 0.32 |
| (3,1142) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HG2 | 10 | 0.32 | 0.04 | 0.32 |
| (3,732) | 1:48:A:ALA:HB2 | 1:43:A:ILE:H | 10 | 0.31 | 0.09 | 0.36 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 10 | 0.31 | 0.09 | 0.36 |
| (3,732) | 1:48:A:ALA:HB3 | 1:43:A:ILE:H | 10 | 0.31 | 0.09 | 0.36 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 10 | 0.31 | 0.14 | 0.31 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 10 | 0.31 | 0.1 | 0.31 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG21 | 10 | 0.31 | 0.1 | 0.31 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG22 | 10 | 0.31 | 0.1 | 0.31 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 10 | 0.31 | 0.13 | 0.28 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 10 | 0.3 | 0.01 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD11 | 10 | 0.3 | 0.01 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD12 | 10 | 0.3 | 0.01 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD13 | 10 | 0.3 | 0.01 | 0.3 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 10 | 0.3 | 0.1 | 0.32 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 10 | 0.3 | 0.0 | 0.3 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 10 | 0.3 | 0.1 | 0.31 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 10 | 0.3 | 0.1 | 0.31 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 10 | 0.3 | 0.1 | 0.31 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 10 | 0.3 | 0.15 | 0.23 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 10 | 0.3 | 0.15 | 0.23 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 10 | 0.3 | 0.15 | 0.23 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 10 | 0.29 | 0.07 | 0.3 |
| (3,1210) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 10 | 0.29 | 0.01 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG22 | 10 | 0.29 | 0.01 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,1210) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG23 | 10 | 0.29 | 0.01 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG23 | 10 | 0.29 | 0.01 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG21 | 10 | 0.29 | 0.01 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG22 | 10 | 0.29 | 0.01 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG23 | 10 | 0.29 | 0.01 | 0.29 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 10 | 0.29 | 0.08 | 0.32 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 10 | 0.28 | 0.01 | 0.28 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 10 | 0.28 | 0.04 | 0.29 |
| (3,1030) | 1:53:A:ILE:H | 1:37:A:ALA:H | 10 | 0.28 | 0.04 | 0.29 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 10 | 0.28 | 0.06 | 0.28 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 10 | 0.28 | 0.06 | 0.28 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 10 | 0.28 | 0.06 | 0.28 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 10 | 0.28 | 0.17 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 10 | 0.28 | 0.17 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 10 | 0.28 | 0.17 | 0.2 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 10 | 0.28 | 0.07 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 10 | 0.28 | 0.09 | 0.28 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 10 | 0.28 | 0.09 | 0.28 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 10 | 0.27 | 0.02 | 0.28 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 10 | 0.27 | 0.07 | 0.28 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 10 | 0.27 | 0.03 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 10 | 0.27 | 0.03 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 10 | 0.27 | 0.03 | 0.27 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 10 | 0.27 | 0.06 | 0.25 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 10 | 0.27 | 0.12 | 0.22 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 10 | 0.27 | 0.08 | 0.23 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 10 | 0.27 | 0.04 | 0.27 |
| (3,423) | 1:61:A:LEU:HD13 | 1:25:A:THR:H | 10 | 0.26 | 0.12 | 0.26 |
| (3,423) | 1:61:A:LEU:HD11 | 1:25:A:THR:H | 10 | 0.26 | 0.12 | 0.26 |
| (3,423) | 1:61:A:LEU:HD12 | 1:25:A:THR:H | 10 | 0.26 | 0.12 | 0.26 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 10 | 0.26 | 0.05 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 10 | 0.26 | 0.0 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 10 | 0.26 | 0.0 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 10 | 0.26 | 0.0 | 0.26 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 10 | 0.26 | 0.02 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 10 | 0.26 | 0.01 | 0.26 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 10 | 0.25 | 0.09 | 0.24 |
| (3,855) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HB2 | 10 | 0.25 | 0.09 | 0.24 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 10 | 0.25 | 0.06 | 0.22 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 10 | 0.25 | 0.06 | 0.22 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 10 | 0.25 | 0.06 | 0.22 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 10 | 0.25 | 0.01 | 0.26 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 10 | 0.25 | 0.07 | 0.23 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 10 | 0.25 | 0.0 | 0.25 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 10 | 0.25 | 0.09 | 0.26 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 10 | 0.25 | 0.09 | 0.26 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 10 | 0.25 | 0.09 | 0.26 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 10 | 0.24 | 0.05 | 0.22 |
| (3,109) | 1:3:A:GLU:HB3 | 1:3:A:GLU:HG2 | 10 | 0.24 | 0.02 | 0.24 |
| (3,109) | 1:4:A:GLU:HB3 | 1:4:A:GLU:HG2 | 10 | 0.24 | 0.02 | 0.24 |
| (3,109) | 1:4:A:GLU:HB3 | 1:4:A:GLU:HG3 | 10 | 0.24 | 0.02 | 0.24 |
| (3,109) | 1:3:A:GLU:HB2 | 1:3:A:GLU:HG3 | 10 | 0.24 | 0.02 | 0.24 |
| (3,109) | 1:2:A:GLU:HB3 | 1:2:A:GLU:HG2 | 10 | 0.24 | 0.02 | 0.24 |
| (3,109) | 1:4:A:GLU:HB2 | 1:4:A:GLU:HG3 | 10 | 0.24 | 0.02 | 0.24 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 10 | 0.24 | 0.02 | 0.25 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 10 | 0.24 | 0.06 | 0.22 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 10 | 0.24 | 0.05 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 10 | 0.24 | 0.05 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 10 | 0.24 | 0.05 | 0.24 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG21 | 10 | 0.24 | 0.07 | 0.22 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG22 | 10 | 0.24 | 0.07 | 0.22 |
| (3,928) | 1:94:A:ILE:HG23 | 1:91:A:LEU:HA | 10 | 0.24 | 0.07 | 0.22 |
| (3,928) | 1:94:A:ILE:HG22 | 1:91:A:LEU:HA | 10 | 0.24 | 0.07 | 0.22 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 10 | 0.23 | 0.04 | 0.24 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 10 | 0.23 | 0.02 | 0.24 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 10 | 0.23 | 0.0 | 0.23 |
| (3,973) | 1:20:A:ILE:HG21 | 1:21:A:VAL:H | 10 | 0.23 | 0.06 | 0.21 |
| (3,973) | 1:20:A:ILE:HG22 | 1:21:A:VAL:H | 10 | 0.23 | 0.06 | 0.21 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 10 | 0.23 | 0.06 | 0.21 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 10 | 0.23 | 0.02 | 0.22 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG23 | 10 | 0.22 | 0.01 | 0.22 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG22 | 10 | 0.22 | 0.01 | 0.22 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG21 | 10 | 0.22 | 0.01 | 0.22 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 10 | 0.22 | 0.09 | 0.18 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 10 | 0.22 | 0.0 | 0.22 |
| (3,864) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 10 | 0.22 | 0.01 | 0.22 |
| (3,864) | 1:53:A:ILE:HG22 | 1:53:A:ILE:HB | 10 | 0.22 | 0.01 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,864) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 10 | 0.22 | 0.01 | 0.22 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 10 | 0.22 | 0.02 | 0.22 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 10 | 0.22 | 0.05 | 0.21 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 10 | 0.22 | 0.05 | 0.21 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 10 | 0.22 | 0.05 | 0.21 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 10 | 0.21 | 0.01 | 0.21 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 10 | 0.21 | 0.04 | 0.22 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 10 | 0.2 | 0.02 | 0.21 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 10 | 0.2 | 0.05 | 0.21 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 10 | 0.2 | 0.05 | 0.21 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 10 | 0.2 | 0.05 | 0.21 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 10 | 0.2 | 0.05 | 0.2 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 10 | 0.2 | 0.03 | 0.19 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 10 | 0.2 | 0.04 | 0.22 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 10 | 0.2 | 0.02 | 0.18 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 10 | 0.2 | 0.07 | 0.18 |
| (3,545) | 1:49:A:VAL:HG12 | 1:49:A:VAL:HA | 10 | 0.19 | 0.03 | 0.18 |
| (3,545) | 1:49:A:VAL:HG13 | 1:49:A:VAL:HA | 10 | 0.19 | 0.03 | 0.18 |
| (3,545) | 1:49:A:VAL:HG11 | 1:49:A:VAL:HA | 10 | 0.19 | 0.03 | 0.18 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 10 | 0.19 | 0.01 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 10 | 0.19 | 0.01 | 0.19 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 10 | 0.18 | 0.04 | 0.2 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 10 | 0.17 | 0.01 | 0.18 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 10 | 0.17 | 0.02 | 0.18 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 10 | 0.17 | 0.04 | 0.19 |
| (3,353) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HB3 | 10 | 0.17 | 0.03 | 0.16 |
| (3,353) | 1:61:A:LEU:HD21 | 1:61:A:LEU:HB3 | 10 | 0.17 | 0.03 | 0.16 |
| (3,353) | 1:61:A:LEU:HD23 | 1:61:A:LEU:HB3 | 10 | 0.17 | 0.03 | 0.16 |
| (3,353) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HB3 | 10 | 0.17 | 0.03 | 0.16 |
| (3,353) | 1:61:A:LEU:HD22 | 1:61:A:LEU:HB3 | 10 | 0.17 | 0.03 | 0.16 |
| (3,353) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HB3 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 10 | 0.17 | 0.03 | 0.17 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 10 | 0.16 | 0.03 | 0.17 |
| (3,268) | 1:125:A:LYS:HE2 | 1:125:A:LYS:HE3 | 10 | 0.16 | 0.0 | 0.16 |
| (3,268) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HE2 | 10 | 0.16 | 0.0 | 0.16 |
| (3,268) | 1:51:A:LYS:HE3 | 1:51:A:LYS:HE2 | 10 | 0.16 | 0.0 | 0.16 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 10 | 0.16 | 0.03 | 0.16 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 10 | 0.16 | 0.01 | 0.16 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD12 | 10 | 0.15 | 0.0 | 0.15 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD13 | 10 | 0.15 | 0.0 | 0.15 |
| (3,321) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HG | 10 | 0.15 | 0.0 | 0.15 |
| (3,321) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HG | 10 | 0.15 | 0.0 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD11 | 10 | 0.15 | 0.0 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 10 | 0.15 | 0.01 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 10 | 0.15 | 0.01 | 0.15 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 10 | 0.14 | 0.01 | 0.15 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG22 | 10 | 0.14 | 0.01 | 0.15 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG23 | 10 | 0.14 | 0.01 | 0.15 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 10 | 0.14 | 0.02 | 0.14 |
| (3,655) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HD3 | 10 | 0.14 | 0.01 | 0.15 |
| (3,655) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HG | 10 | 0.14 | 0.01 | 0.15 |
| (3,655) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HG | 10 | 0.14 | 0.01 | 0.15 |
| (3,655) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HG | 10 | 0.14 | 0.01 | 0.15 |
| (3,655) | 1:26:A:LYS:HG3 | 1:26:A:LYS:HD2 | 10 | 0.14 | 0.01 | 0.15 |
| (3,60) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 10 | 0.14 | 0.01 | 0.14 |
| (3,60) | 1:53:A:ILE:HG22 | 1:53:A:ILE:HB | 10 | 0.14 | 0.01 | 0.14 |
| (3,60) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 10 | 0.14 | 0.01 | 0.14 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 10 | 0.13 | 0.01 | 0.13 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 10 | 0.12 | 0.0 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 10 | 0.12 | 0.01 | 0.12 |
| (3,98) | 1:96:A:GLU:HB3 | 1:96:A:GLU:HB2 | 10 | 0.1 | 0.0 | 0.1 |
| (3,98) | 1:2:A:GLU:HB2 | 1:2:A:GLU:HB3 | 10 | 0.1 | 0.0 | 0.1 |
| (3,98) | 1:3:A:GLU:HB3 | 1:3:A:GLU:HB2 | 10 | 0.1 | 0.0 | 0.1 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 9 | 1.93 | 0.73 | 2.12 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 9 | 1.47 | 0.68 | 1.17 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 9 | 1.2 | 0.04 | 1.19 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 9 | 1.2 | 0.3 | 1.15 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 9 | 1.14 | 0.19 | 1.11 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 9 | 1.06 | 0.06 | 1.08 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 9 | 0.85 | 0.02 | 0.85 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 9 | 0.82 | 0.27 | 0.81 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 9 | 0.8 | 0.08 | 0.77 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 9 | 0.78 | 0.19 | 0.72 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 9 | 0.7 | 0.04 | 0.72 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 9 | 0.6 | 0.13 | 0.57 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,1172) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HG22 | 9 | 0.6 | 0.13 | 0.57 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 9 | 0.6 | 0.31 | 0.51 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 9 | 0.6 | 0.31 | 0.51 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 9 | 0.58 | 0.22 | 0.5 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 9 | 0.57 | 0.14 | 0.5 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 9 | 0.52 | 0.02 | 0.53 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD11 | 9 | 0.51 | 0.19 | 0.55 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD13 | 9 | 0.51 | 0.19 | 0.55 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD12 | 9 | 0.51 | 0.19 | 0.55 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 9 | 0.51 | 0.13 | 0.54 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 9 | 0.48 | 0.32 | 0.41 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 9 | 0.48 | 0.32 | 0.41 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 9 | 0.48 | 0.32 | 0.41 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 9 | 0.48 | 0.11 | 0.47 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 9 | 0.48 | 0.22 | 0.5 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 9 | 0.48 | 0.22 | 0.5 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 9 | 0.48 | 0.08 | 0.5 |
| (3,1157) | 1:80:A:LEU:HD11 | 1:14:A:TRP:HZ3 | 9 | 0.46 | 0.13 | 0.47 |
| (3,1157) | 1:80:A:LEU:HD13 | 1:14:A:TRP:HZ3 | 9 | 0.46 | 0.13 | 0.47 |
| (3,1157) | 1:80:A:LEU:HD12 | 1:14:A:TRP:HZ3 | 9 | 0.46 | 0.13 | 0.47 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 9 | 0.46 | 0.26 | 0.38 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 9 | 0.46 | 0.12 | 0.49 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 9 | 0.45 | 0.16 | 0.45 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 9 | 0.45 | 0.15 | 0.41 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 9 | 0.44 | 0.04 | 0.46 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 9 | 0.44 | 0.21 | 0.39 |
| (3,1164) | 1:28:A:LEU:HD22 | 1:29:A:GLY:H | 9 | 0.44 | 0.21 | 0.39 |
| (3,1164) | 1:28:A:LEU:HD21 | 1:29:A:GLY:H | 9 | 0.44 | 0.21 | 0.39 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 9 | 0.43 | 0.15 | 0.42 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 9 | 0.43 | 0.12 | 0.44 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 9 | 0.41 | 0.13 | 0.37 |
| (3,634) | 1:77:A:ILE:HG12 | 1:104:A:VAL:H | 9 | 0.41 | 0.13 | 0.37 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 9 | 0.39 | 0.12 | 0.39 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 9 | 0.39 | 0.12 | 0.39 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 9 | 0.39 | 0.12 | 0.39 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 9 | 0.39 | 0.02 | 0.38 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 9 | 0.37 | 0.14 | 0.35 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 9 | 0.37 | 0.15 | 0.36 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 9 | 0.35 | 0.08 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 9 | 0.33 | 0.0 | 0.33 |
| (3,843) | 1:75:A:LYS:HB2 | 1:75:A:LYS:HA | 9 | 0.33 | 0.0 | 0.33 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 9 | 0.32 | 0.04 | 0.33 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 9 | 0.32 | 0.09 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 9 | 0.32 | 0.09 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 9 | 0.32 | 0.09 | 0.29 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 9 | 0.31 | 0.02 | 0.32 |
| (3,640) | 1:6:A:LYS:HA | 1:6:A:LYS:H | 9 | 0.31 | 0.02 | 0.32 |
| (3,640) | 1:4:A:GLU:HA | 1:5:A:LYS:H | 9 | 0.31 | 0.02 | 0.32 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 9 | 0.31 | 0.14 | 0.26 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 9 | 0.31 | 0.14 | 0.26 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 9 | 0.31 | 0.09 | 0.29 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 9 | 0.31 | 0.09 | 0.29 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 9 | 0.31 | 0.09 | 0.29 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 9 | 0.31 | 0.1 | 0.28 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 9 | 0.31 | 0.1 | 0.28 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 9 | 0.31 | 0.1 | 0.28 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 9 | 0.3 | 0.1 | 0.26 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 9 | 0.3 | 0.1 | 0.26 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 9 | 0.3 | 0.1 | 0.26 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 9 | 0.3 | 0.1 | 0.29 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 9 | 0.27 | 0.09 | 0.28 |
| (3,885) | 1:69:A:VAL:HG23 | 1:125:A:LYS:HB2 | 9 | 0.27 | 0.03 | 0.28 |
| (3,885) | 1:69:A:VAL:HG21 | 1:69:A:VAL:HB | 9 | 0.27 | 0.03 | 0.28 |
| (3,885) | 1:69:A:VAL:HG21 | 1:125:A:LYS:HB2 | 9 | 0.27 | 0.03 | 0.28 |
| (3,885) | 1:69:A:VAL:HG22 | 1:69:A:VAL:HB | 9 | 0.27 | 0.03 | 0.28 |
| (3,885) | 1:69:A:VAL:HG22 | 1:125:A:LYS:HB2 | 9 | 0.27 | 0.03 | 0.28 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 9 | 0.26 | 0.1 | 0.32 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 9 | 0.26 | 0.1 | 0.32 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 9 | 0.26 | 0.1 | 0.32 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 9 | 0.26 | 0.1 | 0.32 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 9 | 0.26 | 0.1 | 0.32 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 9 | 0.26 | 0.1 | 0.32 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 9 | 0.26 | 0.12 | 0.21 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 9 | 0.26 | 0.12 | 0.21 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 9 | 0.26 | 0.12 | 0.21 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 9 | 0.26 | 0.06 | 0.28 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 9 | 0.26 | 0.06 | 0.28 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 9 | 0.26 | 0.08 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 9 | 0.25 | 0.09 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 9 | 0.25 | 0.09 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 9 | 0.25 | 0.09 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 9 | 0.25 | 0.09 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 9 | 0.25 | 0.09 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 9 | 0.25 | 0.09 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 9 | 0.25 | 0.12 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 9 | 0.25 | 0.12 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 9 | 0.25 | 0.12 | 0.18 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 9 | 0.24 | 0.1 | 0.26 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 9 | 0.24 | 0.09 | 0.22 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD12 | 9 | 0.24 | 0.08 | 0.25 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD11 | 9 | 0.24 | 0.08 | 0.25 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD13 | 9 | 0.24 | 0.08 | 0.25 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 9 | 0.24 | 0.11 | 0.22 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 9 | 0.24 | 0.12 | 0.22 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 9 | 0.24 | 0.12 | 0.22 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 9 | 0.24 | 0.12 | 0.22 |
| (3,129) | 1:77:A:ILE:HD12 | 1:123:A:ILE:HB | 9 | 0.24 | 0.21 | 0.12 |
| (3,129) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HB | 9 | 0.24 | 0.21 | 0.12 |
| (3,129) | 1:77:A:ILE:HG21 | 1:123:A:ILE:HB | 9 | 0.24 | 0.21 | 0.12 |
| (3,129) | 1:77:A:ILE:HD13 | 1:123:A:ILE:HB | 9 | 0.24 | 0.21 | 0.12 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 9 | 0.23 | 0.12 | 0.21 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 9 | 0.23 | 0.05 | 0.23 |
| (3,1128) | 1:72:A:ALA:H | 1:71:A:PRO:HB3 | 9 | 0.23 | 0.07 | 0.23 |
| (3,1128) | 1:75:A:LYS:HG2 | 1:72:A:ALA:H | 9 | 0.23 | 0.07 | 0.23 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 9 | 0.23 | 0.08 | 0.2 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 9 | 0.22 | 0.08 | 0.22 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 9 | 0.22 | 0.08 | 0.22 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 9 | 0.22 | 0.08 | 0.22 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 9 | 0.22 | 0.08 | 0.22 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 9 | 0.22 | 0.04 | 0.23 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 9 | 0.21 | 0.06 | 0.22 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 9 | 0.2 | 0.06 | 0.19 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 9 | 0.19 | 0.05 | 0.22 |
| (3,1182) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 9 | 0.19 | 0.07 | 0.18 |
| (3,1182) | 1:118:A:ILE:HG22 | 1:118:A:ILE:HA | 9 | 0.19 | 0.07 | 0.18 |
| (3,1182) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 9 | 0.19 | 0.07 | 0.18 |
| (3,1182) | 1:98:A:THR:HG22 | 1:98:A:THR:HA | 9 | 0.19 | 0.07 | 0.18 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 9 | 0.18 | 0.04 | 0.18 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 9 | 0.17 | 0.03 | 0.18 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 9 | 0.15 | 0.02 | 0.14 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG22 | 9 | 0.15 | 0.02 | 0.15 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG21 | 9 | 0.15 | 0.02 | 0.15 |
| (3,1057) | 1:8:A:THR:HB | 1:8:A:THR:HG22 | 9 | 0.15 | 0.02 | 0.15 |
| (3,1057) | 1:8:A:THR:HB | 1:8:A:THR:HG21 | 9 | 0.15 | 0.02 | 0.15 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG23 | 9 | 0.15 | 0.02 | 0.15 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 9 | 0.15 | 0.02 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 9 | 0.14 | 0.03 | 0.13 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 9 | 0.14 | 0.03 | 0.13 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 9 | 0.14 | 0.03 | 0.13 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 9 | 0.13 | 0.01 | 0.13 |
| (3,310) | 1:111:A:LYS:HD3 | 1:111:A:LYS:HG2 | 9 | 0.13 | 0.01 | 0.13 |
| (3,310) | 1:111:A:LYS:HD3 | 1:111:A:LYS:HG3 | 9 | 0.13 | 0.01 | 0.13 |
| (3,310) | 1:111:A:LYS:HD2 | 1:111:A:LYS:HG2 | 9 | 0.13 | 0.01 | 0.13 |
| (3,310) | 1:51:A:LYS:HD2 | 1:51:A:LYS:HG3 | 9 | 0.13 | 0.01 | 0.13 |
| (3,310) | 1:111:A:LYS:HD2 | 1:111:A:LYS:HG3 | 9 | 0.13 | 0.01 | 0.13 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 9 | 0.13 | 0.0 | 0.13 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 8 | 1.43 | 0.07 | 1.44 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 8 | 1.38 | 0.71 | 1.6 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 8 | 1.1 | 0.73 | 1.52 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 8 | 1.1 | 0.73 | 1.52 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 8 | 1.1 | 0.73 | 1.52 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 8 | 1.06 | 0.4 | 0.98 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 8 | 1.06 | 0.4 | 0.98 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 8 | 1.06 | 0.4 | 0.98 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 8 | 1.03 | 0.07 | 1.04 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 8 | 0.8 | 0.23 | 0.77 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 8 | 0.8 | 0.23 | 0.77 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 8 | 0.79 | 0.31 | 0.76 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 8 | 0.66 | 0.53 | 0.45 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 8 | 0.65 | 0.34 | 0.63 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 8 | 0.65 | 0.34 | 0.63 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 8 | 0.64 | 0.28 | 0.73 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD3 | 8 | 0.64 | 0.28 | 0.73 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 8 | 0.63 | 0.08 | 0.63 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 8 | 0.62 | 0.11 | 0.65 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 8 | 0.62 | 0.31 | 0.48 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 8 | 0.48 | 0.08 | 0.48 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 8 | 0.47 | 0.17 | 0.48 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 8 | 0.43 | 0.13 | 0.38 |
| (1,2841) | 1:111:A:LYS:HE2 | 1:112:A:GLY:H | 8 | 0.43 | 0.13 | 0.38 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG21 | 8 | 0.41 | 0.16 | 0.4 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 8 | 0.41 | 0.16 | 0.4 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG23 | 8 | 0.41 | 0.16 | 0.4 |
| (3,1087) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HB3 | 8 | 0.41 | 0.17 | 0.38 |
| (3,1087) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HB3 | 8 | 0.41 | 0.17 | 0.38 |
| (3,1087) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HB3 | 8 | 0.41 | 0.17 | 0.38 |
| (3,1087) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HB3 | 8 | 0.41 | 0.17 | 0.38 |
| (3,1087) | 1:61:A:LEU:HD12 | 1:59:A:LEU:HB3 | 8 | 0.41 | 0.17 | 0.38 |
| (3,1087) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HB3 | 8 | 0.41 | 0.17 | 0.38 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 8 | 0.41 | 0.38 | 0.19 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 8 | 0.41 | 0.38 | 0.19 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 8 | 0.41 | 0.38 | 0.19 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 8 | 0.41 | 0.38 | 0.19 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 8 | 0.41 | 0.38 | 0.19 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 8 | 0.41 | 0.38 | 0.19 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 8 | 0.4 | 0.05 | 0.39 |
| (3,366) | 1:42:A:VAL:HG21 | 1:16:A:GLN:HG2 | 8 | 0.37 | 0.19 | 0.31 |
| (3,366) | 1:42:A:VAL:HG23 | 1:16:A:GLN:HG2 | 8 | 0.37 | 0.19 | 0.31 |
| (3,366) | 1:16:A:GLN:HG2 | 1:39:A:VAL:HG12 | 8 | 0.37 | 0.19 | 0.31 |
| (3,366) | 1:42:A:VAL:HG22 | 1:16:A:GLN:HG2 | 8 | 0.37 | 0.19 | 0.31 |
| (3,537) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 8 | 0.36 | 0.13 | 0.35 |
| (3,537) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 8 | 0.36 | 0.13 | 0.35 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 8 | 0.35 | 0.15 | 0.36 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 8 | 0.35 | 0.15 | 0.36 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 8 | 0.35 | 0.15 | 0.36 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 8 | 0.34 | 0.24 | 0.26 |
| (3,165) | 1:79:A:VAL:HG12 | 1:88:A:GLU:HA | 8 | 0.34 | 0.14 | 0.32 |
| (3,165) | 1:79:A:VAL:HG11 | 1:88:A:GLU:HA | 8 | 0.34 | 0.14 | 0.32 |
| (3,165) | 1:79:A:VAL:HG13 | 1:88:A:GLU:HA | 8 | 0.34 | 0.14 | 0.32 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD3 | 8 | 0.34 | 0.04 | 0.35 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 8 | 0.34 | 0.04 | 0.35 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 8 | 0.33 | 0.18 | 0.3 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 8 | 0.32 | 0.16 | 0.26 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 8 | 0.32 | 0.09 | 0.3 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 8 | 0.32 | 0.18 | 0.26 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 8 | 0.32 | 0.18 | 0.26 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 8 | 0.32 | 0.18 | 0.26 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 8 | 0.3 | 0.09 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 8 | 0.3 | 0.09 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 8 | 0.3 | 0.09 | 0.33 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 8 | 0.3 | 0.07 | 0.3 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 8 | 0.29 | 0.12 | 0.26 |
| (3,153) | 1:91:A:LEU:HD11 | 1:102:A:THR:H | 8 | 0.28 | 0.08 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,153) | 1:123:A:ILE:HD13 | 1:102:A:THR:H | 8 | 0.28 | 0.08 | 0.28 |
| (3,153) | 1:123:A:ILE:HD11 | 1:102:A:THR:H | 8 | 0.28 | 0.08 | 0.28 |
| (3,993) | 1:61:A:LEU:HG | 1:50:A:VAL:H | 8 | 0.28 | 0.13 | 0.24 |
| (3,993) | 1:58:A:LYS:HG3 | 1:50:A:VAL:H | 8 | 0.28 | 0.13 | 0.24 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 8 | 0.28 | 0.14 | 0.2 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 8 | 0.28 | 0.14 | 0.2 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 8 | 0.28 | 0.14 | 0.2 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 8 | 0.28 | 0.14 | 0.3 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 8 | 0.26 | 0.16 | 0.2 |
| (1,3245) | 1:30:A:GLU:HG2 | 1:33:A:HIS:H | 8 | 0.26 | 0.12 | 0.26 |
| (1,3245) | 1:30:A:GLU:HG3 | 1:33:A:HIS:H | 8 | 0.26 | 0.12 | 0.26 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 8 | 0.26 | 0.09 | 0.29 |
| (3,595) | 1:105:A:ILE:HB | 1:106:A:GLU:H | 8 | 0.26 | 0.05 | 0.24 |
| (3,595) | 1:106:A:GLU:HG3 | 1:106:A:GLU:H | 8 | 0.26 | 0.05 | 0.24 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 8 | 0.25 | 0.1 | 0.24 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 8 | 0.25 | 0.1 | 0.24 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 8 | 0.25 | 0.1 | 0.24 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 8 | 0.25 | 0.08 | 0.29 |
| (3,743) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HA | 8 | 0.25 | 0.06 | 0.28 |
| (3,743) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HA | 8 | 0.25 | 0.06 | 0.28 |
| (3,743) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HA | 8 | 0.25 | 0.06 | 0.28 |
| (3,296) | 1:91:A:LEU:HD23 | 1:91:A:LEU:HG | 8 | 0.25 | 0.09 | 0.29 |
| (3,296) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 8 | 0.25 | 0.09 | 0.29 |
| (3,296) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB3 | 8 | 0.25 | 0.09 | 0.29 |
| (3,296) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB2 | 8 | 0.25 | 0.09 | 0.29 |
| (3,296) | 1:91:A:LEU:HD22 | 1:91:A:LEU:HG | 8 | 0.25 | 0.09 | 0.29 |
| (3,296) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB3 | 8 | 0.25 | 0.09 | 0.29 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 8 | 0.24 | 0.07 | 0.24 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 8 | 0.23 | 0.09 | 0.22 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 8 | 0.23 | 0.09 | 0.22 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 8 | 0.23 | 0.09 | 0.22 |
| (3,85) | 1:39:A:VAL:HG21 | 1:50:A:VAL:HA | 8 | 0.22 | 0.05 | 0.22 |
| (3,85) | 1:39:A:VAL:HG22 | 1:50:A:VAL:HA | 8 | 0.22 | 0.05 | 0.22 |
| (3,85) | 1:39:A:VAL:HG23 | 1:50:A:VAL:HA | 8 | 0.22 | 0.05 | 0.22 |
| (3,85) | 1:36:A:LYS:HA | 1:69:A:VAL:HG11 | 8 | 0.22 | 0.05 | 0.22 |
| (3,85) | 1:36:A:LYS:HA | 1:69:A:VAL:HG12 | 8 | 0.22 | 0.05 | 0.22 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 8 | 0.21 | 0.05 | 0.2 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 8 | 0.21 | 0.05 | 0.2 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 8 | 0.21 | 0.05 | 0.2 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 8 | 0.21 | 0.06 | 0.18 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 8 | 0.21 | 0.06 | 0.18 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 8 | 0.21 | 0.06 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 8 | 0.2 | 0.07 | 0.2 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 8 | 0.2 | 0.07 | 0.2 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 8 | 0.2 | 0.07 | 0.2 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 8 | 0.2 | 0.11 | 0.16 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 8 | 0.2 | 0.06 | 0.2 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 8 | 0.2 | 0.06 | 0.2 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 8 | 0.2 | 0.06 | 0.2 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 8 | 0.19 | 0.06 | 0.19 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB3 | 8 | 0.19 | 0.06 | 0.19 |
| (3,487) | 1:6:A:LYS:HG2 | 1:6:A:LYS:HE2 | 8 | 0.18 | 0.03 | 0.18 |
| (3,487) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HB | 8 | 0.18 | 0.03 | 0.18 |
| (3,487) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HG3 | 8 | 0.18 | 0.03 | 0.18 |
| (3,487) | 1:5:A:LYS:HG2 | 1:5:A:LYS:HE3 | 8 | 0.18 | 0.03 | 0.18 |
| (3,487) | 1:5:A:LYS:HE2 | 1:5:A:LYS:HG3 | 8 | 0.18 | 0.03 | 0.18 |
| (3,487) | 1:6:A:LYS:HG3 | 1:6:A:LYS:HE2 | 8 | 0.18 | 0.03 | 0.18 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 8 | 0.18 | 0.04 | 0.18 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 8 | 0.18 | 0.04 | 0.18 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 8 | 0.18 | 0.04 | 0.18 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 8 | 0.17 | 0.06 | 0.15 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 8 | 0.17 | 0.06 | 0.15 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 8 | 0.17 | 0.06 | 0.15 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 8 | 0.16 | 0.04 | 0.17 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 8 | 0.15 | 0.03 | 0.15 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 8 | 0.14 | 0.02 | 0.14 |
| (3,729) | 1:26:A:LYS:HE2 | 1:26:A:LYS:HD3 | 8 | 0.12 | 0.01 | 0.12 |
| (3,729) | 1:26:A:LYS:HD2 | 1:26:A:LYS:HE3 | 8 | 0.12 | 0.01 | 0.12 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 7 | 2.61 | 0.32 | 2.52 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 7 | 1.29 | 0.51 | 1.12 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 7 | 0.97 | 0.66 | 0.71 |
| (3,564) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 7 | 0.97 | 0.24 | 1.07 |
| (3,564) | 1:34:A:LYS:HE2 | 1:34:A:LYS:HG2 | 7 | 0.97 | 0.24 | 1.07 |
| (3,564) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 7 | 0.97 | 0.24 | 1.07 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 7 | 0.96 | 0.16 | 0.98 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 7 | 0.78 | 0.01 | 0.78 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 7 | 0.78 | 0.5 | 1.11 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 7 | 0.73 | 0.33 | 0.61 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 7 | 0.73 | 0.33 | 0.61 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 7 | 0.73 | 0.33 | 0.61 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 7 | 0.61 | 0.3 | 0.63 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 7 | 0.61 | 0.3 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 7 | 0.61 | 0.3 | 0.63 |
| (1,1606) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 7 | 0.59 | 0.0 | 0.59 |
| (1,1606) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 7 | 0.59 | 0.0 | 0.59 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 7 | 0.58 | 0.04 | 0.56 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG23 | 7 | 0.57 | 0.35 | 0.53 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG21 | 7 | 0.57 | 0.35 | 0.53 |
| (3,1097) | 1:82:A:GLY:H | 1:79:A:VAL:HG21 | 7 | 0.57 | 0.35 | 0.53 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG22 | 7 | 0.57 | 0.35 | 0.53 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 7 | 0.53 | 0.27 | 0.51 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 7 | 0.53 | 0.27 | 0.51 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 7 | 0.53 | 0.27 | 0.51 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE2 | 7 | 0.5 | 0.19 | 0.51 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE3 | 7 | 0.5 | 0.19 | 0.51 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 7 | 0.5 | 0.06 | 0.5 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 7 | 0.49 | 0.23 | 0.58 |
| (3,300) | 1:11:A:THR:HG21 | 1:13:A:TYR:HE1 | 7 | 0.47 | 0.15 | 0.51 |
| (3,300) | 1:11:A:THR:HG23 | 1:13:A:TYR:HE2 | 7 | 0.47 | 0.15 | 0.51 |
| (3,300) | 1:11:A:THR:HG22 | 1:13:A:TYR:HE2 | 7 | 0.47 | 0.15 | 0.51 |
| (3,300) | 1:11:A:THR:HG23 | 1:13:A:TYR:HE1 | 7 | 0.47 | 0.15 | 0.51 |
| (3,300) | 1:11:A:THR:HG22 | 1:13:A:TYR:HE1 | 7 | 0.47 | 0.15 | 0.51 |
| (3,849) | 1:26:A:LYS:HB3 | 1:33:A:HIS:H | 7 | 0.46 | 0.09 | 0.5 |
| (3,849) | 1:35:A:LYS:HD2 | 1:33:A:HIS:H | 7 | 0.46 | 0.09 | 0.5 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 7 | 0.46 | 0.01 | 0.46 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 7 | 0.45 | 0.16 | 0.52 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 7 | 0.43 | 0.1 | 0.48 |
| (3,378) | 1:89:A:GLY:H | 1:105:A:ILE:HD13 | 7 | 0.43 | 0.1 | 0.48 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 7 | 0.43 | 0.19 | 0.46 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 7 | 0.42 | 0.02 | 0.42 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 7 | 0.41 | 0.0 | 0.41 |
| (1,1484) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 7 | 0.41 | 0.01 | 0.41 |
| (1,1484) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 7 | 0.41 | 0.01 | 0.41 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 7 | 0.39 | 0.27 | 0.27 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 7 | 0.37 | 0.26 | 0.2 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 7 | 0.37 | 0.21 | 0.33 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 7 | 0.36 | 0.23 | 0.26 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 7 | 0.35 | 0.13 | 0.43 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 7 | 0.34 | 0.18 | 0.26 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 7 | 0.33 | 0.28 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 7 | 0.33 | 0.28 | 0.23 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 7 | 0.32 | 0.14 | 0.29 |
| (3,1108) | 1:10:A:ARG:HB3 | 1:81:A:ASN:HD21 | 7 | 0.32 | 0.14 | 0.29 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 7 | 0.32 | 0.16 | 0.42 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 7 | 0.31 | 0.16 | 0.32 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 7 | 0.31 | 0.16 | 0.32 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 7 | 0.31 | 0.16 | 0.32 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 7 | 0.31 | 0.01 | 0.31 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 7 | 0.3 | 0.27 | 0.19 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 7 | 0.3 | 0.08 | 0.33 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 7 | 0.29 | 0.11 | 0.3 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 7 | 0.28 | 0.06 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 7 | 0.28 | 0.06 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 7 | 0.28 | 0.06 | 0.26 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 7 | 0.27 | 0.09 | 0.27 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 7 | 0.27 | 0.04 | 0.26 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 7 | 0.26 | 0.11 | 0.23 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 7 | 0.25 | 0.1 | 0.23 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 7 | 0.25 | 0.1 | 0.23 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 7 | 0.25 | 0.1 | 0.23 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 7 | 0.24 | 0.08 | 0.21 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 7 | 0.23 | 0.18 | 0.14 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 7 | 0.22 | 0.07 | 0.22 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 7 | 0.21 | 0.02 | 0.21 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 7 | 0.21 | 0.06 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 7 | 0.21 | 0.06 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 7 | 0.21 | 0.06 | 0.19 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 7 | 0.21 | 0.0 | 0.21 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 7 | 0.2 | 0.08 | 0.2 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 7 | 0.19 | 0.06 | 0.2 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 7 | 0.19 | 0.06 | 0.2 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 7 | 0.19 | 0.06 | 0.2 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 7 | 0.19 | 0.06 | 0.16 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 7 | 0.19 | 0.06 | 0.16 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 7 | 0.19 | 0.06 | 0.16 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 7 | 0.18 | 0.08 | 0.14 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 7 | 0.18 | 0.06 | 0.18 |
| (3,144) | 1:96:A:GLU:HB3 | 1:97:A:LYS:H | 7 | 0.18 | 0.06 | 0.18 |
| (3,1167) | 1:115:A:VAL:HG23 | 1:115:A:VAL:HB | 7 | 0.13 | 0.01 | 0.13 |
| (3,1167) | 1:115:A:VAL:HG22 | 1:115:A:VAL:HB | 7 | 0.13 | 0.01 | 0.13 |
| (3,1167) | 1:115:A:VAL:HG21 | 1:115:A:VAL:HB | 7 | 0.13 | 0.01 | 0.13 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 7 | 0.12 | 0.01 | 0.11 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 7 | 0.11 | 0.0 | 0.11 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 6 | 1.93 | 0.8 | 2.3 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 6 | 1.93 | 0.8 | 2.3 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 6 | 1.93 | 0.8 | 2.3 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 6 | 1.52 | 0.19 | 1.5 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 6 | 1.37 | 0.63 | 1.66 |
| (3,31) | 1:75:A:LYS:HE2 | 1:76:A:ARG:H | 6 | 1.16 | 0.17 | 1.16 |
| (3,31) | 1:75:A:LYS:HE3 | 1:76:A:ARG:H | 6 | 1.16 | 0.17 | 1.16 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 6 | 1.15 | 0.58 | 1.03 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 6 | 1.15 | 0.58 | 1.03 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 6 | 1.15 | 0.58 | 1.03 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 6 | 1.1 | 0.62 | 0.97 |
| (3,563) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 6 | 1.05 | 0.01 | 1.05 |
| (3,563) | 1:58:A:LYS:HG2 | 1:58:A:LYS:HE2 | 6 | 1.05 | 0.01 | 1.05 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 6 | 0.95 | 0.02 | 0.95 |
| (1,3758) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 6 | 0.92 | 0.48 | 0.72 |
| (1,3758) | 1:65:A:HIS:HE1 | 1:27:A:LYS:HD2 | 6 | 0.92 | 0.48 | 0.72 |
| (3,518) | 1:26:A:LYS:HD2 | 1:30:A:GLU:HG2 | 6 | 0.67 | 0.45 | 0.54 |
| (3,518) | 1:96:A:GLU:HG3 | 1:97:A:LYS:HG3 | 6 | 0.67 | 0.45 | 0.54 |
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 6 | 0.65 | 0.32 | 0.48 |
| (3,339) | 1:30:A:GLU:HG3 | 1:32:A:TYR:H | 6 | 0.63 | 0.12 | 0.64 |
| (3,339) | 1:30:A:GLU:HG2 | 1:32:A:TYR:H | 6 | 0.63 | 0.12 | 0.64 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 6 | 0.56 | 0.29 | 0.52 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 6 | 0.55 | 0.03 | 0.55 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 6 | 0.53 | 0.65 | 0.28 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 6 | 0.53 | 0.65 | 0.28 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 6 | 0.53 | 0.65 | 0.28 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 6 | 0.49 | 0.16 | 0.45 |
| (3,583) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB3 | 6 | 0.47 | 0.27 | 0.5 |
| (3,583) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB3 | 6 | 0.47 | 0.27 | 0.5 |
| (3,583) | 1:125:A:LYS:HE2 | 1:20:A:ILE:HD12 | 6 | 0.47 | 0.27 | 0.5 |
| (3,583) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB3 | 6 | 0.47 | 0.27 | 0.5 |
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 6 | 0.42 | 0.06 | 0.42 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 6 | 0.41 | 0.05 | 0.38 |
| (3,1076) | 1:5:A:LYS:H | 1:5:A:LYS:HD3 | 6 | 0.38 | 0.19 | 0.3 |
| (3,1076) | 1:97:A:LYS:H | 1:97:A:LYS:HD3 | 6 | 0.38 | 0.19 | 0.3 |
| (3,1076) | 1:97:A:LYS:H | 1:97:A:LYS:HD2 | 6 | 0.38 | 0.19 | 0.3 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD11 | 6 | 0.33 | 0.3 | 0.22 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD12 | 6 | 0.33 | 0.3 | 0.22 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD13 | 6 | 0.33 | 0.3 | 0.22 |
| (3,4) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 6 | 0.3 | 0.09 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,4) | 1:102:A:THR:HG23 | 1:116:A:GLU:H | 6 | 0.3 | 0.09 | 0.29 |
| (3,4) | 1:102:A:THR:HG22 | 1:116:A:GLU:H | 6 | 0.3 | 0.09 | 0.29 |
| (1,3163) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 6 | 0.3 | 0.09 | 0.34 |
| (1,3163) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 6 | 0.3 | 0.09 | 0.34 |
| (1,3163) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 6 | 0.3 | 0.09 | 0.34 |
| (1,3163) | 1:49:A:VAL:HG11 | 1:41:A:GLU:H | 6 | 0.3 | 0.09 | 0.34 |
| (1,3163) | 1:49:A:VAL:HG12 | 1:41:A:GLU:H | 6 | 0.3 | 0.09 | 0.34 |
| (1,3163) | 1:49:A:VAL:HG13 | 1:41:A:GLU:H | 6 | 0.3 | 0.09 | 0.34 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 6 | 0.29 | 0.16 | 0.26 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 6 | 0.29 | 0.14 | 0.29 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 6 | 0.29 | 0.14 | 0.29 |
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 6 | 0.29 | 0.14 | 0.29 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 6 | 0.29 | 0.15 | 0.28 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 6 | 0.29 | 0.15 | 0.28 |
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 6 | 0.29 | 0.15 | 0.28 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 6 | 0.28 | 0.24 | 0.18 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD12 | 6 | 0.28 | 0.07 | 0.25 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD11 | 6 | 0.28 | 0.07 | 0.25 |
| (3,680) | 1:64:A:THR:H | 1:24:A:ILE:HD11 | 6 | 0.28 | 0.07 | 0.25 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 6 | 0.28 | 0.12 | 0.3 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 6 | 0.25 | 0.21 | 0.18 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 6 | 0.25 | 0.21 | 0.18 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 6 | 0.25 | 0.21 | 0.18 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 6 | 0.25 | 0.11 | 0.24 |
| (3,440) | 1:93:A:SER:H | 1:103:A:ILE:H | 6 | 0.24 | 0.08 | 0.22 |
| (3,440) | 1:103:A:ILE:H | 1:117:A:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 6 | 0.23 | 0.06 | 0.24 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 6 | 0.23 | 0.1 | 0.22 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 6 | 0.23 | 0.1 | 0.22 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 6 | 0.23 | 0.1 | 0.22 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 6 | 0.22 | 0.14 | 0.18 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 6 | 0.22 | 0.14 | 0.18 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 6 | 0.22 | 0.13 | 0.17 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 6 | 0.22 | 0.13 | 0.17 |
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 6 | 0.22 | 0.13 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 6 | 0.21 | 0.1 | 0.2 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 6 | 0.2 | 0.04 | 0.22 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 6 | 0.2 | 0.1 | 0.16 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 6 | 0.2 | 0.1 | 0.16 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 6 | 0.2 | 0.1 | 0.16 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 6 | 0.19 | 0.05 | 0.18 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 6 | 0.18 | 0.09 | 0.15 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 6 | 0.18 | 0.09 | 0.15 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 6 | 0.18 | 0.09 | 0.15 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 6 | 0.18 | 0.07 | 0.16 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 6 | 0.18 | 0.07 | 0.16 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 6 | 0.18 | 0.07 | 0.16 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 6 | 0.17 | 0.02 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 6 | 0.17 | 0.02 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 6 | 0.17 | 0.02 | 0.18 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 6 | 0.17 | 0.04 | 0.16 |
| (3,690) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 6 | 0.16 | 0.0 | 0.16 |
| (3,690) | 1:58:A:LYS:HG2 | 1:58:A:LYS:HE2 | 6 | 0.16 | 0.0 | 0.16 |
| (3,890) | 1:78:A:LEU:HA | 1:124:A:SER:H | 6 | 0.16 | 0.04 | 0.15 |
| (3,890) | 1:68:A:THR:HB | 1:124:A:SER:H | 6 | 0.16 | 0.04 | 0.15 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 6 | 0.16 | 0.03 | 0.15 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 6 | 0.14 | 0.03 | 0.15 |
| (3,332) | 1:43:A:ILE:HG21 | 1:43:A:ILE:HG13 | 6 | 0.13 | 0.02 | 0.13 |
| (3,332) | 1:43:A:ILE:HG22 | 1:43:A:ILE:HG13 | 6 | 0.13 | 0.02 | 0.13 |
| (3,332) | 1:43:A:ILE:HG23 | 1:43:A:ILE:HG13 | 6 | 0.13 | 0.02 | 0.13 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 6 | 0.12 | 0.02 | 0.11 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 6 | 0.12 | 0.01 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 6 | 0.12 | 0.01 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 6 | 0.12 | 0.01 | 0.12 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG11 | 5 | 1.9 | 0.04 | 1.89 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG12 | 5 | 1.9 | 0.04 | 1.89 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG13 | 5 | 1.9 | 0.04 | 1.89 |
| (1,1926) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 5 | 1.38 | 0.13 | 1.38 |
| (1,1926) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 5 | 1.38 | 0.13 | 1.38 |
| (1,1926) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 5 | 1.38 | 0.13 | 1.38 |
| (3,317) | 1:34:A:LYS:HB3 | 1:34:A:LYS:HE2 | 5 | 1.29 | 0.11 | 1.29 |
| (3,317) | 1:34:A:LYS:HB2 | 1:34:A:LYS:HE2 | 5 | 1.29 | 0.11 | 1.29 |
| (3,317) | 1:34:A:LYS:HE3 | 1:34:A:LYS:HB3 | 5 | 1.29 | 0.11 | 1.29 |
| (1,2420) | 1:115:A:VAL:HG21 | 1:118:A:ILE:H | 5 | 1.24 | 0.1 | 1.28 |
| (1,2420) | 1:115:A:VAL:HG22 | 1:118:A:ILE:H | 5 | 1.24 | 0.1 | 1.28 |
| (1,2420) | 1:115:A:VAL:HG23 | 1:118:A:ILE:H | 5 | 1.24 | 0.1 | 1.28 |
| (1,2432) | 1:115:A:VAL:HG21 | 1:116:A:GLU:H | 5 | 1.23 | 0.05 | 1.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2432) | 1:115:A:VAL:HG22 | 1:116:A:GLU:H | 5 | 1.23 | 0.05 | 1.23 |
| (1,2432) | 1:115:A:VAL:HG23 | 1:116:A:GLU:H | 5 | 1.23 | 0.05 | 1.23 |
| (1,2533) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 5 | 1.21 | 0.09 | 1.26 |
| (1,2533) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 5 | 1.21 | 0.09 | 1.26 |
| (1,2533) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 5 | 1.21 | 0.09 | 1.26 |
| (1,1921) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 5 | 1.18 | 0.09 | 1.15 |
| (1,1921) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 5 | 1.18 | 0.09 | 1.15 |
| (1,1921) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 5 | 1.18 | 0.09 | 1.15 |
| (1,1751) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 5 | 1.09 | 0.1 | 1.11 |
| (1,1751) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 5 | 1.09 | 0.1 | 1.11 |
| (1,1751) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 5 | 1.09 | 0.1 | 1.11 |
| (1,2163) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HA | 5 | 1.05 | 0.07 | 1.07 |
| (1,2163) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HA | 5 | 1.05 | 0.07 | 1.07 |
| (1,2163) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HA | 5 | 1.05 | 0.07 | 1.07 |
| (1,834) | 1:52:A:MET:HG2 | 1:59:A:LEU:HG | 5 | 1.0 | 0.45 | 1.23 |
| (1,1927) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 5 | 0.97 | 0.1 | 0.99 |
| (1,1927) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 5 | 0.97 | 0.1 | 0.99 |
| (1,1927) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 5 | 0.97 | 0.1 | 0.99 |
| (1,1915) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 5 | 0.95 | 0.01 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 5 | 0.95 | 0.01 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 5 | 0.95 | 0.01 | 0.95 |
| (1,1886) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 5 | 0.88 | 0.09 | 0.85 |
| (1,1886) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 5 | 0.88 | 0.09 | 0.85 |
| (1,1886) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 5 | 0.88 | 0.09 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG11 | 5 | 0.87 | 0.09 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG12 | 5 | 0.87 | 0.09 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG13 | 5 | 0.87 | 0.09 | 0.85 |
| (1,3557) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HD21 | 5 | 0.87 | 0.83 | 0.43 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 5 | 0.86 | 0.15 | 0.86 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 5 | 0.86 | 0.15 | 0.86 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 5 | 0.86 | 0.15 | 0.86 |
| (3,857) | 1:115:A:VAL:HG13 | 1:114:A:ARG:HB2 | 5 | 0.81 | 0.15 | 0.82 |
| (3,857) | 1:114:A:ARG:HB3 | 1:115:A:VAL:HG13 | 5 | 0.81 | 0.15 | 0.82 |
| (3,857) | 1:114:A:ARG:HB3 | 1:115:A:VAL:HG11 | 5 | 0.81 | 0.15 | 0.82 |
| (3,241) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HE22 | 5 | 0.79 | 0.26 | 0.77 |
| (1,1933) | 1:115:A:VAL:HG21 | 1:116:A:GLU:HA | 5 | 0.75 | 0.03 | 0.75 |
| (1,1933) | 1:115:A:VAL:HG22 | 1:116:A:GLU:HA | 5 | 0.75 | 0.03 | 0.75 |
| (1,1933) | 1:115:A:VAL:HG23 | 1:116:A:GLU:HA | 5 | 0.75 | 0.03 | 0.75 |
| (1,3331) | 1:20:A:ILE:H | 1:124:A:SER:HB3 | 5 | 0.72 | 0.14 | 0.7 |
| (3,177) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HA | 5 | 0.62 | 0.32 | 0.76 |
| (3,177) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 5 | 0.62 | 0.32 | 0.76 |
| (1,1258) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 5 | 0.6 | 0.47 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1919) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 5 | 0.58 | 0.0 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 5 | 0.58 | 0.0 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 5 | 0.58 | 0.0 | 0.58 |
| (1,1262) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 5 | 0.57 | 0.47 | 0.34 |
| (1,2450) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 5 | 0.55 | 0.01 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 5 | 0.55 | 0.01 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 5 | 0.55 | 0.01 | 0.55 |
| (1,3648) | 1:16:A:GLN:HE22 | 1:80:A:LEU:HG | 5 | 0.55 | 0.2 | 0.5 |
| (1,42) | 1:8:A:THR:HA | 1:9:A:ALA:H | 5 | 0.54 | 0.15 | 0.56 |
| (1,290) | 1:20:A:ILE:HG13 | 1:127:A:ALA:HA | 5 | 0.49 | 0.13 | 0.42 |
| (1,2162) | 1:115:A:VAL:HG21 | 1:113:A:ARG:HD3 | 5 | 0.47 | 0.07 | 0.45 |
| (1,2162) | 1:115:A:VAL:HG22 | 1:113:A:ARG:HD3 | 5 | 0.47 | 0.07 | 0.45 |
| (1,2162) | 1:115:A:VAL:HG23 | 1:113:A:ARG:HD3 | 5 | 0.47 | 0.07 | 0.45 |
| (1,3641) | 1:11:A:THR:H | 1:81:A:ASN:HD21 | 5 | 0.47 | 0.35 | 0.37 |
| (1,2221) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HA | 5 | 0.47 | 0.52 | 0.19 |
| (1,2221) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HA | 5 | 0.47 | 0.52 | 0.19 |
| (1,2221) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 5 | 0.47 | 0.52 | 0.19 |
| (1,3726) | 1:95:A:ASN:HD21 | 1:98:A:THR:HB | 5 | 0.46 | 0.25 | 0.35 |
| (1,3714) | 1:84:A:TYR:HD1 | 1:87:A:ASN:HD22 | 5 | 0.44 | 0.14 | 0.44 |
| (1,3714) | 1:84:A:TYR:HD2 | 1:87:A:ASN:HD22 | 5 | 0.44 | 0.14 | 0.44 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 5 | 0.44 | 0.49 | 0.19 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 5 | 0.44 | 0.49 | 0.19 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 5 | 0.44 | 0.49 | 0.19 |
| (2,142) | 1:10:A:ARG:HA | 1:82:A:GLY:HA3 | 5 | 0.43 | 0.14 | 0.38 |
| (1,2456) | 1:115:A:VAL:HG11 | 1:114:A:ARG:H | 5 | 0.43 | 0.03 | 0.41 |
| (1,2456) | 1:115:A:VAL:HG12 | 1:114:A:ARG:H | 5 | 0.43 | 0.03 | 0.41 |
| (1,2456) | 1:115:A:VAL:HG13 | 1:114:A:ARG:H | 5 | 0.43 | 0.03 | 0.41 |
| (1,816) | 1:111:A:LYS:HD3 | 1:106:A:GLU:HA | 5 | 0.41 | 0.09 | 0.43 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 5 | 0.39 | 0.15 | 0.39 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 5 | 0.39 | 0.15 | 0.39 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 5 | 0.39 | 0.15 | 0.39 |
| (3,1137) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 5 | 0.39 | 0.21 | 0.25 |
| (3,628) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 5 | 0.38 | 0.0 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 5 | 0.38 | 0.0 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 5 | 0.38 | 0.0 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 5 | 0.38 | 0.0 | 0.38 |
| (1,3434) | 1:63:A:GLN:HE22 | 1:14:A:TRP:HE1 | 5 | 0.37 | 0.17 | 0.4 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG21 | 5 | 0.37 | 0.14 | 0.44 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG22 | 5 | 0.37 | 0.14 | 0.44 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG23 | 5 | 0.37 | 0.14 | 0.44 |
| (1,3715) | 1:84:A:TYR:HE1 | 1:87:A:ASN:HD22 | 5 | 0.34 | 0.16 | 0.31 |
| (1,3715) | 1:84:A:TYR:HE2 | 1:87:A:ASN:HD22 | 5 | 0.34 | 0.16 | 0.31 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3403) | 1:10:A:ARG:HD2 | 1:10:A:ARG:H | 5 | 0.34 | 0.16 | 0.35 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD11 | 5 | 0.33 | 0.11 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD12 | 5 | 0.33 | 0.11 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD13 | 5 | 0.33 | 0.11 | 0.32 |
| (1,25) | 1:7:A:ARG:HA | 1:7:A:ARG:HG2 | 5 | 0.32 | 0.04 | 0.31 |
| (1,3128) | 1:47:A:THR:HB | 1:44:A:ASP:H | 5 | 0.29 | 0.11 | 0.23 |
| (1,281) | 1:20:A:ILE:HD11 | 1:20:A:ILE:HB | 5 | 0.29 | 0.33 | 0.13 |
| (1,281) | 1:20:A:ILE:HD12 | 1:20:A:ILE:HB | 5 | 0.29 | 0.33 | 0.13 |
| (1,281) | 1:20:A:ILE:HD13 | 1:20:A:ILE:HB | 5 | 0.29 | 0.33 | 0.13 |
| (2,574) | 1:39:A:VAL:H | 1:20:A:ILE:HG12 | 5 | 0.28 | 0.1 | 0.25 |
| (1,2205) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 5 | 0.28 | 0.06 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 5 | 0.28 | 0.06 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 5 | 0.28 | 0.06 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG11 | 1:41:A:GLU:H | 5 | 0.28 | 0.06 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG12 | 1:41:A:GLU:H | 5 | 0.28 | 0.06 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG13 | 1:41:A:GLU:H | 5 | 0.28 | 0.06 | 0.31 |
| (1,693) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 5 | 0.28 | 0.11 | 0.25 |
| (1,693) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 5 | 0.28 | 0.11 | 0.25 |
| (1,693) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 5 | 0.28 | 0.11 | 0.25 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 5 | 0.28 | 0.22 | 0.16 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 5 | 0.28 | 0.22 | 0.16 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 5 | 0.28 | 0.22 | 0.16 |
| (3,280) | 1:112:A:GLY:H | 1:111:A:LYS:HG3 | 5 | 0.26 | 0.11 | 0.28 |
| (1,3737) | 1:5:A:LYS:H | 1:3:A:GLU:H | 5 | 0.25 | 0.13 | 0.21 |
| (3,613) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 5 | 0.25 | 0.0 | 0.25 |
| (3,1091) | 1:112:A:GLY:H | 1:105:A:ILE:H | 5 | 0.25 | 0.08 | 0.25 |
| (3,1091) | 1:115:A:VAL:H | 1:105:A:ILE:H | 5 | 0.25 | 0.08 | 0.25 |
| (1,2633) | 1:96:A:GLU:H | 1:95:A:ASN:HB3 | 5 | 0.23 | 0.07 | 0.27 |
| (1,2461) | 1:84:A:TYR:HE1 | 1:113:A:ARG:H | 5 | 0.23 | 0.12 | 0.2 |
| (1,2461) | 1:84:A:TYR:HE2 | 1:113:A:ARG:H | 5 | 0.23 | 0.12 | 0.2 |
| (1,2447) | 1:115:A:VAL:HB | 1:115:A:VAL:H | 5 | 0.22 | 0.04 | 0.19 |
| (3,1170) | 1:111:A:LYS:HB2 | 1:112:A:GLY:H | 5 | 0.22 | 0.06 | 0.23 |
| (1,683) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HA | 5 | 0.22 | 0.06 | 0.23 |
| (1,683) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HA | 5 | 0.22 | 0.06 | 0.23 |
| (1,683) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HA | 5 | 0.22 | 0.06 | 0.23 |
| (1,3000) | 1:59:A:LEU:HD11 | 1:60:A:LYS:H | 5 | 0.21 | 0.08 | 0.23 |
| (1,3000) | 1:59:A:LEU:HD12 | 1:60:A:LYS:H | 5 | 0.21 | 0.08 | 0.23 |
| (1,3000) | 1:59:A:LEU:HD13 | 1:60:A:LYS:H | 5 | 0.21 | 0.08 | 0.23 |
| (1,2285) | 1:20:A:ILE:HA | 1:20:A:ILE:HG12 | 5 | 0.21 | 0.0 | 0.21 |
| (1,3631) | 1:23:A:ILE:H | 1:32:A:TYR:HB3 | 5 | 0.2 | 0.1 | 0.13 |
| (1,1492) | 1:104:A:VAL:H | 1:90:A:THR:HB | 5 | 0.19 | 0.13 | 0.15 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG21 | 5 | 0.19 | 0.03 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG22 | 5 | 0.19 | 0.03 | 0.18 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG23 | 5 | 0.19 | 0.03 | 0.18 |
| (1,900) | 1:57:A:ASP:HA | 1:57:A:ASP:HB3 | 5 | 0.19 | 0.02 | 0.2 |
| (3,838) | 1:52:A:MET:H | 1:59:A:LEU:H | 5 | 0.19 | 0.06 | 0.16 |
| (3,838) | 1:53:A:ILE:H | 1:52:A:MET:H | 5 | 0.19 | 0.06 | 0.16 |
| (3,854) | 1:104:A:VAL:HA | 1:103:A:ILE:HB | 5 | 0.19 | 0.04 | 0.17 |
| (3,180) | 1:65:A:HIS:H | 1:62:A:ASP:HB3 | 5 | 0.18 | 0.03 | 0.2 |
| (3,396) | 1:118:A:ILE:HG23 | 1:121:A:GLU:HA | 5 | 0.18 | 0.05 | 0.18 |
| (3,396) | 1:121:A:GLU:HA | 1:123:A:ILE:HG22 | 5 | 0.18 | 0.05 | 0.18 |
| (3,396) | 1:118:A:ILE:HG22 | 1:121:A:GLU:HA | 5 | 0.18 | 0.05 | 0.18 |
| (1,1352) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA2 | 5 | 0.18 | 0.04 | 0.16 |
| (1,1352) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA2 | 5 | 0.18 | 0.04 | 0.16 |
| (1,1352) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA2 | 5 | 0.18 | 0.04 | 0.16 |
| (1,1021) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 5 | 0.17 | 0.05 | 0.16 |
| (1,1021) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 5 | 0.17 | 0.05 | 0.16 |
| (1,1021) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 5 | 0.17 | 0.05 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 5 | 0.16 | 0.06 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 5 | 0.16 | 0.06 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 5 | 0.16 | 0.06 | 0.16 |
| (1,154) | 1:16:A:GLN:HA | 1:16:A:GLN:HB3 | 5 | 0.16 | 0.01 | 0.17 |
| (1,3134) | 1:44:A:ASP:H | 1:43:A:ILE:HG13 | 5 | 0.15 | 0.05 | 0.12 |
| (1,530) | 1:37:A:ALA:HB1 | 1:38:A:ILE:H | 5 | 0.15 | 0.04 | 0.13 |
| (1,530) | 1:37:A:ALA:HB2 | 1:38:A:ILE:H | 5 | 0.15 | 0.04 | 0.13 |
| (1,530) | 1:37:A:ALA:HB3 | 1:38:A:ILE:H | 5 | 0.15 | 0.04 | 0.13 |
| (1,3537) | 1:46:A:TYR:HE1 | 1:63:A:GLN:HE21 | 5 | 0.15 | 0.02 | 0.16 |
| (1,3537) | 1:46:A:TYR:HE2 | 1:63:A:GLN:HE21 | 5 | 0.15 | 0.02 | 0.16 |
| (1,2967) | 1:46:A:TYR:HB2 | 1:63:A:GLN:H | 5 | 0.15 | 0.04 | 0.15 |
| (1,1611) | 1:98:A:THR:HA | 1:98:A:THR:HB | 5 | 0.14 | 0.02 | 0.14 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 5 | 0.14 | 0.02 | 0.14 |
| (3,450) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 5 | 0.14 | 0.04 | 0.12 |
| (3,450) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 5 | 0.14 | 0.04 | 0.12 |
| (1,479) | 1:31:A:LYS:HA | 1:32:A:TYR:H | 5 | 0.14 | 0.01 | 0.13 |
| (3,817) | 1:84:A:TYR:HA | 1:85:A:ARG:H | 5 | 0.14 | 0.02 | 0.13 |
| (1,2218) | 1:102:A:THR:HB | 1:103:A:ILE:H | 5 | 0.13 | 0.01 | 0.14 |
| (1,439) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 5 | 0.13 | 0.01 | 0.13 |
| (1,2509) | 1:107:A:THR:H | 1:88:A:GLU:H | 5 | 0.12 | 0.03 | 0.11 |
| (1,1785) | 1:107:A:THR:HB | 1:107:A:THR:HA | 5 | 0.11 | 0.01 | 0.11 |
| (1,861) | 1:53:A:ILE:HD11 | 1:36:A:LYS:HE2 | 4 | 1.51 | 0.87 | 1.72 |
| (1,861) | 1:53:A:ILE:HD12 | 1:36:A:LYS:HE2 | 4 | 1.51 | 0.87 | 1.72 |
| (1,861) | 1:53:A:ILE:HD13 | 1:36:A:LYS:HE2 | 4 | 1.51 | 0.87 | 1.72 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,861) | 1:53:A:ILE:HD11 | 1:36:A:LYS:HE3 | 4 | 1.51 | 0.87 | 1.72 |
| (1,861) | 1:53:A:ILE:HD12 | 1:36:A:LYS:HE3 | 4 | 1.51 | 0.87 | 1.72 |
| (1,861) | 1:53:A:ILE:HD13 | 1:36:A:LYS:HE3 | 4 | 1.51 | 0.87 | 1.72 |
| (2,344) | 1:81:A:ASN:HB3 | 1:123:A:ILE:HA | 4 | 1.16 | 0.1 | 1.17 |
| (1,1197) | 1:75:A:LYS:HE3 | 1:71:A:PRO:HB2 | 4 | 1.05 | 0.3 | 1.0 |
| (3,186) | 1:52:A:MET:HG3 | 1:59:A:LEU:H | 4 | 1.04 | 0.56 | 1.18 |
| (3,186) | 1:59:A:LEU:H | 1:57:A:ASP:HB2 | 4 | 1.04 | 0.56 | 1.18 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG21 | 4 | 0.97 | 1.33 | 0.22 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG22 | 4 | 0.97 | 1.33 | 0.22 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG23 | 4 | 0.97 | 1.33 | 0.22 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG21 | 4 | 0.97 | 1.33 | 0.22 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG22 | 4 | 0.97 | 1.33 | 0.22 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG23 | 4 | 0.97 | 1.33 | 0.22 |
| (1,3421) | 1:10:A:ARG:H | 1:82:A:GLY:HA3 | 4 | 0.96 | 0.59 | 0.96 |
| (1,14) | 1:5:A:LYS:HA | 1:5:A:LYS:HD2 | 4 | 0.93 | 0.5 | 1.08 |
| (1,14) | 1:5:A:LYS:HA | 1:5:A:LYS:HD3 | 4 | 0.93 | 0.5 | 1.08 |
| (3,876) | 1:10:A:ARG:HD3 | 1:81:A:ASN:HD21 | 4 | 0.83 | 0.3 | 0.88 |
| (3,876) | 1:10:A:ARG:HD2 | 1:81:A:ASN:HD21 | 4 | 0.83 | 0.3 | 0.88 |
| (2,611) | 1:123:A:ILE:H | 1:81:A:ASN:HB3 | 4 | 0.81 | 0.21 | 0.86 |
| (1,2773) | 1:10:A:ARG:HG2 | 1:83:A:GLY:H | 4 | 0.8 | 0.26 | 0.73 |
| (1,1898) | 1:115:A:VAL:H | 1:114:A:ARG:HG2 | 4 | 0.78 | 0.47 | 0.72 |
| (1,467) | 1:30:A:GLU:HG2 | 1:30:A:GLU:HA | 4 | 0.78 | 0.01 | 0.78 |
| (3,961) | 1:30:A:GLU:HG2 | 1:29:A:GLY:H | 4 | 0.75 | 0.46 | 0.52 |
| (3,125) | 1:44:A:ASP:HB2 | 1:46:A:TYR:HD1 | 4 | 0.68 | 0.36 | 0.6 |
| (3,125) | 1:44:A:ASP:HB2 | 1:46:A:TYR:HD2 | 4 | 0.68 | 0.36 | 0.6 |
| (3,125) | 1:13:A:TYR:HD2 | 1:45:A:LYS:HE3 | 4 | 0.68 | 0.36 | 0.6 |
| (3,125) | 1:13:A:TYR:HD1 | 1:45:A:LYS:HE3 | 4 | 0.68 | 0.36 | 0.6 |
| (1,3652) | 1:22:A:LYS:H | 1:22:A:LYS:HE2 | 4 | 0.63 | 0.19 | 0.7 |
| (3,122) | 1:44:A:ASP:HB3 | 1:43:A:ILE:HG22 | 4 | 0.59 | 0.39 | 0.48 |
| (3,122) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HG23 | 4 | 0.59 | 0.39 | 0.48 |
| (3,122) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HG21 | 4 | 0.59 | 0.39 | 0.48 |
| (3,122) | 1:44:A:ASP:HB3 | 1:43:A:ILE:HG21 | 4 | 0.59 | 0.39 | 0.48 |
| (1,3509) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 4 | 0.58 | 0.32 | 0.55 |
| (3,582) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 4 | 0.56 | 0.08 | 0.59 |
| (3,582) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 4 | 0.56 | 0.08 | 0.59 |
| (1,3414) | 1:4:A:GLU:H | 1:3:A:GLU:H | 4 | 0.54 | 0.2 | 0.54 |
| (1,2792) | 1:81:A:ASN:H | 1:81:A:ASN:HB3 | 4 | 0.52 | 0.04 | 0.51 |
| (1,3453) | 1:14:A:TRP:HA | 1:16:A:GLN:HE22 | 4 | 0.5 | 0.44 | 0.31 |
| (1,3599) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD22 | 4 | 0.5 | 0.18 | 0.44 |
| (1,3599) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD22 | 4 | 0.5 | 0.18 | 0.44 |
| (1,3599) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD22 | 4 | 0.5 | 0.18 | 0.44 |
| (1,287) | 1:20:A:ILE:HD11 | 1:20:A:ILE:H | 4 | 0.46 | 0.04 | 0.46 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,287) | 1:20:A:ILE:HD12 | 1:20:A:ILE:H | 4 | 0.46 | 0.04 | 0.46 |
| (1,287) | 1:20:A:ILE:HD13 | 1:20:A:ILE:H | 4 | 0.46 | 0.04 | 0.46 |
| (3,379) | 1:45:A:LYS:HA | 1:46:A:TYR:HD2 | 4 | 0.45 | 0.32 | 0.44 |
| (3,379) | 1:45:A:LYS:HA | 1:13:A:TYR:HD2 | 4 | 0.45 | 0.32 | 0.44 |
| (3,379) | 1:45:A:LYS:HA | 1:13:A:TYR:HD1 | 4 | 0.45 | 0.32 | 0.44 |
| (1,2621) | 1:97:A:LYS:H | 1:97:A:LYS:HD3 | 4 | 0.41 | 0.28 | 0.3 |
| (1,2621) | 1:97:A:LYS:H | 1:97:A:LYS:HD2 | 4 | 0.41 | 0.28 | 0.3 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG11 | 4 | 0.37 | 0.06 | 0.36 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG12 | 4 | 0.37 | 0.06 | 0.36 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG13 | 4 | 0.37 | 0.06 | 0.36 |
| (1,2636) | 1:96:A:GLU:H | 1:97:A:LYS:HD3 | 4 | 0.34 | 0.25 | 0.28 |
| (1,2636) | 1:96:A:GLU:H | 1:97:A:LYS:HD2 | 4 | 0.34 | 0.25 | 0.28 |
| (1,3753) | 1:34:A:LYS:HD2 | 1:33:A:HIS:HE1 | 4 | 0.32 | 0.15 | 0.26 |
| (1,3695) | 1:68:A:THR:H | 1:121:A:GLU:HB3 | 4 | 0.32 | 0.09 | 0.34 |
| (1,3695) | 1:68:A:THR:H | 1:121:A:GLU:HB2 | 4 | 0.32 | 0.09 | 0.34 |
| (3,345) | 1:35:A:LYS:H | 1:22:A:LYS:HG3 | 4 | 0.32 | 0.08 | 0.34 |
| (1,3591) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD21 | 4 | 0.31 | 0.2 | 0.21 |
| (1,3591) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD21 | 4 | 0.31 | 0.2 | 0.21 |
| (1,3591) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD21 | 4 | 0.31 | 0.2 | 0.21 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 4 | 0.3 | 0.13 | 0.29 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 4 | 0.3 | 0.13 | 0.29 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 4 | 0.3 | 0.13 | 0.29 |
| (1,3449) | 1:15:A:LEU:H | 1:14:A:TRP:HE1 | 4 | 0.29 | 0.16 | 0.28 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG21 | 4 | 0.29 | 0.09 | 0.28 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG22 | 4 | 0.29 | 0.09 | 0.28 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG23 | 4 | 0.29 | 0.09 | 0.28 |
| (1,2157) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB3 | 4 | 0.27 | 0.17 | 0.18 |
| (1,458) | 1:61:A:LEU:HD21 | 1:60:A:LYS:H | 4 | 0.26 | 0.15 | 0.22 |
| (1,458) | 1:61:A:LEU:HD22 | 1:60:A:LYS:H | 4 | 0.26 | 0.15 | 0.22 |
| (1,458) | 1:61:A:LEU:HD23 | 1:60:A:LYS:H | 4 | 0.26 | 0.15 | 0.22 |
| (1,2047) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 4 | 0.26 | 0.07 | 0.24 |
| (1,2047) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 4 | 0.26 | 0.07 | 0.24 |
| (1,2047) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 4 | 0.26 | 0.07 | 0.24 |
| (1,3243) | 1:30:A:GLU:HB3 | 1:33:A:HIS:H | 4 | 0.25 | 0.12 | 0.18 |
| (1,3243) | 1:30:A:GLU:HB2 | 1:33:A:HIS:H | 4 | 0.25 | 0.12 | 0.18 |
| (3,1174) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD2 | 4 | 0.25 | 0.05 | 0.26 |
| (2,609) | 1:119:A:GLN:HE21 | 1:121:A:GLU:HB2 | 4 | 0.23 | 0.04 | 0.22 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 4 | 0.22 | 0.08 | 0.2 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 4 | 0.22 | 0.08 | 0.2 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 4 | 0.22 | 0.08 | 0.2 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG11 | 4 | 0.22 | 0.06 | 0.2 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG12 | 4 | 0.22 | 0.06 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG13 | 4 | 0.22 | 0.06 | 0.2 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD11 | 4 | 0.22 | 0.06 | 0.2 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD12 | 4 | 0.22 | 0.06 | 0.2 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD13 | 4 | 0.22 | 0.06 | 0.2 |
| (1,375) | 1:23:A:ILE:HG21 | 1:66:A:LEU:HA | 4 | 0.22 | 0.08 | 0.2 |
| (1,375) | 1:23:A:ILE:HG22 | 1:66:A:LEU:HA | 4 | 0.22 | 0.08 | 0.2 |
| (1,375) | 1:23:A:ILE:HG23 | 1:66:A:LEU:HA | 4 | 0.22 | 0.08 | 0.2 |
| (3,303) | 1:102:A:THR:HA | 1:103:A:ILE:HD11 | 4 | 0.21 | 0.06 | 0.21 |
| (3,303) | 1:102:A:THR:HA | 1:103:A:ILE:HD13 | 4 | 0.21 | 0.06 | 0.21 |
| (2,626) | 1:48:A:ALA:H | 1:60:A:LYS:HE3 | 4 | 0.2 | 0.08 | 0.2 |
| (1,2197) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 4 | 0.19 | 0.06 | 0.17 |
| (1,906) | 1:58:A:LYS:H | 1:57:A:ASP:HB2 | 4 | 0.18 | 0.04 | 0.18 |
| (3,69) | 1:66:A:LEU:HD13 | 1:21:A:VAL:HB | 4 | 0.18 | 0.08 | 0.14 |
| (3,69) | 1:66:A:LEU:HD11 | 1:21:A:VAL:HB | 4 | 0.18 | 0.08 | 0.14 |
| (3,69) | 1:66:A:LEU:HD12 | 1:21:A:VAL:HB | 4 | 0.18 | 0.08 | 0.14 |
| (1,1997) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 4 | 0.18 | 0.03 | 0.16 |
| (1,1966) | 1:118:A:ILE:HG21 | 1:122:A:ASP:H | 4 | 0.18 | 0.04 | 0.18 |
| (1,1966) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 4 | 0.18 | 0.04 | 0.18 |
| (1,1966) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 4 | 0.18 | 0.04 | 0.18 |
| (1,1223) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 4 | 0.18 | 0.05 | 0.18 |
| (1,1616) | 1:98:A:THR:HG21 | 1:98:A:THR:H | 4 | 0.18 | 0.05 | 0.18 |
| (1,1616) | 1:98:A:THR:HG22 | 1:98:A:THR:H | 4 | 0.18 | 0.05 | 0.18 |
| (1,1616) | 1:98:A:THR:HG23 | 1:98:A:THR:H | 4 | 0.18 | 0.05 | 0.18 |
| (1,2641) | 1:95:A:ASN:HD21 | 1:95:A:ASN:H | 4 | 0.18 | 0.08 | 0.15 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG11 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG12 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG13 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG11 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG12 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG13 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG11 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG12 | 4 | 0.18 | 0.07 | 0.16 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG13 | 4 | 0.18 | 0.07 | 0.16 |
| (3,128) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HG23 | 4 | 0.18 | 0.06 | 0.17 |
| (3,128) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 4 | 0.18 | 0.06 | 0.17 |
| (3,128) | 1:77:A:ILE:HD12 | 1:123:A:ILE:HG22 | 4 | 0.18 | 0.06 | 0.17 |
| (3,128) | 1:77:A:ILE:HD13 | 1:123:A:ILE:HG21 | 4 | 0.18 | 0.06 | 0.17 |
| (1,248) | 1:19:A:ILE:HD11 | 1:14:A:TRP:HZ3 | 4 | 0.17 | 0.05 | 0.16 |
| (1,248) | 1:19:A:ILE:HD12 | 1:14:A:TRP:HZ3 | 4 | 0.17 | 0.05 | 0.16 |
| (1,248) | 1:19:A:ILE:HD13 | 1:14:A:TRP:HZ3 | 4 | 0.17 | 0.05 | 0.16 |
| (1,1777) | 1:106:A:GLU:HB3 | 1:106:A:GLU:H | 4 | 0.16 | 0.04 | 0.16 |
| (1,3705) | 1:75:A:LYS:H | 1:91:A:LEU:HA | 4 | 0.16 | 0.04 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG11 | 4 | 0.15 | 0.03 | 0.15 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG12 | 4 | 0.15 | 0.03 | 0.15 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG13 | 4 | 0.15 | 0.03 | 0.15 |
| (3,816) | 1:77:A:ILE:H | 1:91:A:LEU:H | 4 | 0.15 | 0.03 | 0.15 |
| (1,3752) | 1:34:A:LYS:HG2 | 1:33:A:HIS:HE1 | 4 | 0.15 | 0.04 | 0.14 |
| (1,1716) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 4 | 0.14 | 0.04 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG22 | 1:102:A:THR:HA | 4 | 0.14 | 0.04 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 4 | 0.14 | 0.04 | 0.12 |
| (1,1386) | 1:81:A:ASN:HA | 1:81:A:ASN:HB2 | 4 | 0.14 | 0.01 | 0.15 |
| (1,2049) | 1:19:A:ILE:HB | 1:124:A:SER:HB2 | 4 | 0.13 | 0.01 | 0.14 |
| (1,288) | 1:20:A:ILE:H | 1:20:A:ILE:HG12 | 4 | 0.12 | 0.01 | 0.11 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD11 | 4 | 0.12 | 0.02 | 0.11 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD12 | 4 | 0.12 | 0.02 | 0.11 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD13 | 4 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:7:A:ARG:HA | 1:7:A:ARG:HD3 | 3 | 1.28 | 0.05 | 1.27 |
| (1,48) | 1:3:A:GLU:HB2 | 1:8:A:THR:HB | 3 | 1.18 | 0.09 | 1.24 |
| (1,48) | 1:3:A:GLU:HB3 | 1:8:A:THR:HB | 3 | 1.18 | 0.09 | 1.24 |
| (3,1140) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 3 | 0.95 | 0.19 | 1.06 |
| (3,780) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 3 | 0.85 | 0.51 | 1.21 |
| (1,59) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 3 | 0.84 | 0.28 | 0.86 |
| (3,1144) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 3 | 0.81 | 0.19 | 0.92 |
| (1,2591) | 1:95:A:ASN:HB2 | 1:100:A:SER:H | 3 | 0.77 | 0.25 | 0.6 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG21 | 3 | 0.75 | 0.35 | 0.99 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG22 | 3 | 0.75 | 0.35 | 0.99 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG23 | 3 | 0.75 | 0.35 | 0.99 |
| (1,3061) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 3 | 0.71 | 0.03 | 0.72 |
| (1,2239) | 1:10:A:ARG:HG2 | 1:82:A:GLY:HA3 | 3 | 0.64 | 0.46 | 0.49 |
| (3,32) | 1:22:A:LYS:HD2 | 1:34:A:LYS:HA | 3 | 0.61 | 0.04 | 0.63 |
| (3,32) | 1:34:A:LYS:HA | 1:34:A:LYS:HD2 | 3 | 0.61 | 0.04 | 0.63 |
| (3,560) | 1:31:A:LYS:HG3 | 1:33:A:HIS:H | 3 | 0.59 | 0.22 | 0.72 |
| (3,560) | 1:34:A:LYS:HG3 | 1:33:A:HIS:H | 3 | 0.59 | 0.22 | 0.72 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB1 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB2 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB3 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB1 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB2 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB3 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB1 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB2 | 3 | 0.59 | 0.46 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 3 | 0.59 | 0.46 | 0.4 |
| (1,3560) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 3 | 0.55 | 0.28 | 0.57 |
| (1,2604) | 1:95:A:ASN:HB2 | 1:99:A:PHE:H | 3 | 0.54 | 0.34 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,414) | 1:22:A:LYS:HD2 | 1:34:A:LYS:HA | 3 | 0.53 | 0.04 | 0.56 |
| (3,414) | 1:34:A:LYS:HA | 1:34:A:LYS:HD2 | 3 | 0.53 | 0.04 | 0.56 |
| (3,1181) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 3 | 0.51 | 0.13 | 0.51 |
| (1,829) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 3 | 0.48 | 0.0 | 0.48 |
| (3,975) | 1:97:A:LYS:HB2 | 1:98:A:THR:HG22 | 3 | 0.47 | 0.17 | 0.54 |
| (3,975) | 1:97:A:LYS:HB2 | 1:98:A:THR:HG21 | 3 | 0.47 | 0.17 | 0.54 |
| (3,975) | 1:77:A:ILE:HB | 1:123:A:ILE:HG21 | 3 | 0.47 | 0.17 | 0.54 |
| (1,2158) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 3 | 0.47 | 0.1 | 0.53 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE1 | 3 | 0.46 | 0.17 | 0.35 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE2 | 3 | 0.46 | 0.17 | 0.35 |
| (1,739) | 1:45:A:LYS:HG2 | 1:45:A:LYS:HE2 | 3 | 0.45 | 0.02 | 0.45 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD11 | 3 | 0.44 | 0.38 | 0.22 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD12 | 3 | 0.44 | 0.38 | 0.22 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD13 | 3 | 0.44 | 0.38 | 0.22 |
| (1,3725) | 1:95:A:ASN:HD22 | 1:95:A:ASN:H | 3 | 0.44 | 0.04 | 0.41 |
| (1,3493) | 1:26:A:LYS:HB2 | 1:33:A:HIS:H | 3 | 0.42 | 0.32 | 0.21 |
| (2,589) | 1:82:A:GLY:HA3 | 1:11:A:THR:H | 3 | 0.4 | 0.15 | 0.33 |
| (3,1183) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 3 | 0.38 | 0.13 | 0.39 |
| (3,919) | 1:65:A:HIS:HE1 | 1:27:A:LYS:HD2 | 3 | 0.36 | 0.16 | 0.46 |
| (3,919) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 3 | 0.36 | 0.16 | 0.46 |
| (3,919) | 1:75:A:LYS:HD3 | 1:72:A:ALA:H | 3 | 0.36 | 0.16 | 0.46 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD11 | 3 | 0.35 | 0.15 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD12 | 3 | 0.35 | 0.15 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD13 | 3 | 0.35 | 0.15 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD11 | 3 | 0.35 | 0.15 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD12 | 3 | 0.35 | 0.15 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD13 | 3 | 0.35 | 0.15 | 0.36 |
| (1,3592) | 1:95:A:ASN:HA | 1:95:A:ASN:HD22 | 3 | 0.35 | 0.1 | 0.3 |
| (1,2865) | 1:75:A:LYS:H | 1:71:A:PRO:HB2 | 3 | 0.34 | 0.33 | 0.11 |
| (1,2494) | 1:108:A:GLY:H | 1:111:A:LYS:HE3 | 3 | 0.33 | 0.14 | 0.27 |
| (3,21) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HG2 | 3 | 0.32 | 0.16 | 0.27 |
| (3,21) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HG2 | 3 | 0.32 | 0.16 | 0.27 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD11 | 3 | 0.32 | 0.07 | 0.36 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD12 | 3 | 0.32 | 0.07 | 0.36 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD13 | 3 | 0.32 | 0.07 | 0.36 |
| (3,782) | 1:96:A:GLU:HB3 | 1:94:A:ILE:HD11 | 3 | 0.32 | 0.07 | 0.36 |
| (3,782) | 1:96:A:GLU:HB3 | 1:94:A:ILE:HD12 | 3 | 0.32 | 0.07 | 0.36 |
| (3,782) | 1:96:A:GLU:HB3 | 1:94:A:ILE:HD13 | 3 | 0.32 | 0.07 | 0.36 |
| (1,2880) | 1:75:A:LYS:HB3 | 1:72:A:ALA:H | 3 | 0.31 | 0.23 | 0.17 |
| (3,1221) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HD11 | 3 | 0.31 | 0.12 | 0.36 |
| (3,1221) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HD13 | 3 | 0.31 | 0.12 | 0.36 |
| (3,1221) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HD11 | 3 | 0.31 | 0.12 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG21 | 3 | 0.3 | 0.14 | 0.21 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG22 | 3 | 0.3 | 0.14 | 0.21 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG23 | 3 | 0.3 | 0.14 | 0.21 |
| (1,1896) | 1:114:A:ARG:HA | 1:114:A:ARG:HG2 | 3 | 0.3 | 0.13 | 0.38 |
| (1,3656) | 1:32:A:TYR:HB2 | 1:27:A:LYS:H | 3 | 0.3 | 0.2 | 0.16 |
| (2,650) | 1:61:A:LEU:HB2 | 1:65:A:HIS:HD2 | 3 | 0.29 | 0.22 | 0.18 |
| (3,1184) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 3 | 0.28 | 0.13 | 0.29 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG21 | 3 | 0.28 | 0.13 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG22 | 3 | 0.28 | 0.13 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG23 | 3 | 0.28 | 0.13 | 0.19 |
| (1,3126) | 1:44:A:ASP:H | 1:47:A:THR:HA | 3 | 0.28 | 0.04 | 0.28 |
| (3,23) | 1:127:A:ALA:HB3 | 1:18:A:GLU:H | 3 | 0.27 | 0.06 | 0.29 |
| (3,23) | 1:127:A:ALA:HB2 | 1:18:A:GLU:H | 3 | 0.27 | 0.06 | 0.29 |
| (3,23) | 1:127:A:ALA:HB1 | 1:18:A:GLU:H | 3 | 0.27 | 0.06 | 0.29 |
| (3,348) | 1:7:A:ARG:HD2 | 1:7:A:ARG:H | 3 | 0.27 | 0.06 | 0.31 |
| (3,348) | 1:113:A:ARG:H | 1:113:A:ARG:HD2 | 3 | 0.27 | 0.06 | 0.31 |
| (1,832) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 3 | 0.26 | 0.03 | 0.27 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG21 | 3 | 0.26 | 0.08 | 0.24 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG22 | 3 | 0.26 | 0.08 | 0.24 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG23 | 3 | 0.26 | 0.08 | 0.24 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD11 | 3 | 0.25 | 0.09 | 0.22 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD12 | 3 | 0.25 | 0.09 | 0.22 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD13 | 3 | 0.25 | 0.09 | 0.22 |
| (1,2571) | 1:117:A:GLY:HA2 | 1:101:A:ALA:H | 3 | 0.25 | 0.16 | 0.17 |
| (1,3391) | 1:11:A:THR:H | 1:81:A:ASN:HD22 | 3 | 0.25 | 0.04 | 0.26 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG21 | 3 | 0.24 | 0.09 | 0.3 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG22 | 3 | 0.24 | 0.09 | 0.3 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG23 | 3 | 0.24 | 0.09 | 0.3 |
| (1,2137) | 1:119:A:GLN:HG2 | 1:100:A:SER:HB2 | 3 | 0.23 | 0.05 | 0.22 |
| (2,617) | 1:24:A:ILE:HA | 1:33:A:HIS:H | 3 | 0.23 | 0.03 | 0.24 |
| (1,1638) | 1:118:A:ILE:H | 1:100:A:SER:HB2 | 3 | 0.22 | 0.1 | 0.18 |
| (3,489) | 1:82:A:GLY:HA3 | 1:81:A:ASN:HB3 | 3 | 0.22 | 0.09 | 0.23 |
| (3,489) | 1:51:A:LYS:HE3 | 1:56:A:GLY:HA3 | 3 | 0.22 | 0.09 | 0.23 |
| (3,140) | 1:78:A:LEU:HD21 | 1:88:A:GLU:HG3 | 3 | 0.21 | 0.06 | 0.19 |
| (3,140) | 1:78:A:LEU:HD22 | 1:88:A:GLU:HG3 | 3 | 0.21 | 0.06 | 0.19 |
| (3,140) | 1:24:A:ILE:HG21 | 1:67:A:GLU:HG2 | 3 | 0.21 | 0.06 | 0.19 |
| (1,3133) | 1:44:A:ASP:H | 1:43:A:ILE:HG12 | 3 | 0.21 | 0.04 | 0.19 |
| (1,3468) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HE21 | 3 | 0.2 | 0.02 | 0.21 |
| (1,3468) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HE21 | 3 | 0.2 | 0.02 | 0.21 |
| (1,3468) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HE21 | 3 | 0.2 | 0.02 | 0.21 |
| (1,2788) | 1:81:A:ASN:H | 1:84:A:TYR:H | 3 | 0.2 | 0.09 | 0.16 |
| (1,3021) | 1:51:A:LYS:HD2 | 1:57:A:ASP:H | 3 | 0.2 | 0.03 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1971) | 1:119:A:GLN:HA | 1:101:A:ALA:H | 3 | 0.19 | 0.04 | 0.17 |
| (1,1) | 1:107:A:THR:HB | 1:108:A:GLY:H | 3 | 0.19 | 0.07 | 0.17 |
| (1,2339) | 1:77:A:ILE:HA | 1:124:A:SER:H | 3 | 0.19 | 0.03 | 0.18 |
| (1,2193) | 1:107:A:THR:HG21 | 1:87:A:ASN:HA | 3 | 0.18 | 0.09 | 0.12 |
| (1,2193) | 1:107:A:THR:HG22 | 1:87:A:ASN:HA | 3 | 0.18 | 0.09 | 0.12 |
| (1,2193) | 1:107:A:THR:HG23 | 1:87:A:ASN:HA | 3 | 0.18 | 0.09 | 0.12 |
| (3,523) | 1:20:A:ILE:HG22 | 1:127:A:ALA:HA | 3 | 0.18 | 0.01 | 0.17 |
| (1,2831) | 1:78:A:LEU:H | 1:123:A:ILE:HB | 3 | 0.17 | 0.02 | 0.17 |
| (1,1138) | 1:79:A:VAL:HG11 | 1:87:A:ASN:HB3 | 3 | 0.17 | 0.01 | 0.17 |
| (1,1138) | 1:79:A:VAL:HG12 | 1:87:A:ASN:HB3 | 3 | 0.17 | 0.01 | 0.17 |
| (1,1138) | 1:79:A:VAL:HG13 | 1:87:A:ASN:HB3 | 3 | 0.17 | 0.01 | 0.17 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD11 | 3 | 0.16 | 0.04 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD12 | 3 | 0.16 | 0.04 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD13 | 3 | 0.16 | 0.04 | 0.19 |
| (1,2448) | 1:115:A:VAL:H | 1:103:A:ILE:HG13 | 3 | 0.16 | 0.04 | 0.13 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD11 | 3 | 0.16 | 0.04 | 0.13 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD12 | 3 | 0.16 | 0.04 | 0.13 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD13 | 3 | 0.16 | 0.04 | 0.13 |
| (3,1146) | 1:115:A:VAL:HA | 1:103:A:ILE:H | 3 | 0.15 | 0.02 | 0.14 |
| (1,1678) | 1:102:A:THR:HG21 | 1:103:A:ILE:HA | 3 | 0.14 | 0.02 | 0.14 |
| (1,1678) | 1:102:A:THR:HG22 | 1:103:A:ILE:HA | 3 | 0.14 | 0.02 | 0.14 |
| (1,1678) | 1:102:A:THR:HG23 | 1:103:A:ILE:HA | 3 | 0.14 | 0.02 | 0.14 |
| (1,922) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 3 | 0.14 | 0.03 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB1 | 1:42:A:VAL:H | 3 | 0.14 | 0.0 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB2 | 1:42:A:VAL:H | 3 | 0.14 | 0.0 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB3 | 1:42:A:VAL:H | 3 | 0.14 | 0.0 | 0.14 |
| (1,1946) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HB3 | 3 | 0.13 | 0.03 | 0.12 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG21 | 3 | 0.13 | 0.02 | 0.12 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.12 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.12 |
| (1,1441) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,1947) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HA | 3 | 0.13 | 0.03 | 0.11 |
| (1,2368) | 1:119:A:GLN:HA | 1:121:A:GLU:H | 3 | 0.12 | 0.01 | 0.13 |
| (1,788) | 1:49:A:VAL:HG21 | 1:48:A:ALA:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,788) | 1:49:A:VAL:HG22 | 1:48:A:ALA:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,788) | 1:49:A:VAL:HG23 | 1:48:A:ALA:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,3213) | 1:36:A:LYS:H | 1:35:A:LYS:H | 3 | 0.11 | 0.01 | 0.12 |
| (3,534) | 1:82:A:GLY:H | 1:81:A:ASN:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,28) | 1:7:A:ARG:HB2 | 1:7:A:ARG:HG3 | 3 | 0.1 | 0.0 | 0.1 |
| (1,28) | 1:7:A:ARG:HB3 | 1:7:A:ARG:HG2 | 3 | 0.1 | 0.0 | 0.1 |
| (1,963) | 1:34:A:LYS:HE2 | 1:33:A:HIS:HE1 | 2 | 1.64 | 0.38 | 1.64 |
| (1,2096) | 1:125:A:LYS:HE2 | 1:127:A:ALA:HA | 2 | 1.62 | 0.82 | 1.62 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3755) | 1:34:A:LYS:HE2 | 1:33:A:HIS:HE1 | 2 | 1.54 | 0.38 | 1.54 |
| (1,2107) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HB3 | 2 | 1.35 | 0.1 | 1.35 |
| (1,2107) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HB3 | 2 | 1.35 | 0.1 | 1.35 |
| (1,2107) | 1:126:A:LEU:HD23 | 1:88:A:GLU:HB3 | 2 | 1.35 | 0.1 | 1.35 |
| (1,1790) | 1:107:A:THR:HG21 | 1:88:A:GLU:HG3 | 2 | 1.26 | 0.02 | 1.26 |
| (1,1790) | 1:107:A:THR:HG22 | 1:88:A:GLU:HG3 | 2 | 1.26 | 0.02 | 1.26 |
| (1,1790) | 1:107:A:THR:HG23 | 1:88:A:GLU:HG3 | 2 | 1.26 | 0.02 | 1.26 |
| (3,1179) | 1:27:A:LYS:HA | 1:27:A:LYS:HD2 | 2 | 1.26 | 0.02 | 1.26 |
| (1,452) | 1:28:A:LEU:HD11 | 1:60:A:LYS:H | 2 | 1.23 | 0.1 | 1.23 |
| (1,452) | 1:28:A:LEU:HD12 | 1:60:A:LYS:H | 2 | 1.23 | 0.1 | 1.23 |
| (1,452) | 1:28:A:LEU:HD13 | 1:60:A:LYS:H | 2 | 1.23 | 0.1 | 1.23 |
| (1,2720) | 1:88:A:GLU:HG3 | 1:88:A:GLU:H | 2 | 1.16 | 0.04 | 1.16 |
| (1,1317) | 1:31:A:LYS:HG2 | 1:32:A:TYR:H | 2 | 1.05 | 0.03 | 1.05 |
| (1,3253) | 1:31:A:LYS:HG2 | 1:32:A:TYR:H | 2 | 1.02 | 0.03 | 1.02 |
| (1,3837) | 1:11:A:THR:HB | 1:13:A:TYR:HE1 | 2 | 1.0 | 0.01 | 1.0 |
| (1,3837) | 1:11:A:THR:HB | 1:13:A:TYR:HE2 | 2 | 1.0 | 0.01 | 1.0 |
| (1,2697) | 1:106:A:GLU:HG2 | 1:90:A:THR:H | 2 | 1.0 | 0.26 | 1.0 |
| (1,75) | 1:11:A:THR:HB | 1:13:A:TYR:HD1 | 2 | 0.97 | 0.12 | 0.97 |
| (1,75) | 1:11:A:THR:HB | 1:13:A:TYR:HD2 | 2 | 0.97 | 0.12 | 0.97 |
| (3,555) | 1:12:A:ASP:HB2 | 1:46:A:TYR:HE2 | 2 | 0.95 | 0.68 | 0.95 |
| (1,426) | 1:91:A:LEU:HD21 | 1:102:A:THR:H | 2 | 0.94 | 0.78 | 0.94 |
| (1,426) | 1:91:A:LEU:HD22 | 1:102:A:THR:H | 2 | 0.94 | 0.78 | 0.94 |
| (1,426) | 1:91:A:LEU:HD23 | 1:102:A:THR:H | 2 | 0.94 | 0.78 | 0.94 |
| (3,635) | 1:23:A:ILE:HG22 | 1:24:A:ILE:H | 2 | 0.92 | 0.09 | 0.92 |
| (1,170) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HG3 | 2 | 0.91 | 0.47 | 0.91 |
| (1,170) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HG3 | 2 | 0.91 | 0.47 | 0.91 |
| (1,170) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HG3 | 2 | 0.91 | 0.47 | 0.91 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG21 | 2 | 0.88 | 0.2 | 0.88 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG22 | 2 | 0.88 | 0.2 | 0.88 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG23 | 2 | 0.88 | 0.2 | 0.88 |
| (1,1729) | 1:106:A:GLU:HG2 | 1:105:A:ILE:HA | 2 | 0.86 | 0.12 | 0.86 |
| (2,365) | 1:107:A:THR:HB | 1:88:A:GLU:HG3 | 2 | 0.84 | 0.01 | 0.84 |
| (2,366) | 1:107:A:THR:HB | 1:88:A:GLU:HG3 | 2 | 0.84 | 0.01 | 0.84 |
| (1,1617) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 2 | 0.8 | 0.0 | 0.8 |
| (1,1617) | 1:98:A:THR:HG22 | 1:98:A:THR:HA | 2 | 0.8 | 0.0 | 0.8 |
| (1,1617) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 2 | 0.8 | 0.0 | 0.8 |
| (2,590) | 1:7:A:ARG:HB2 | 1:9:A:ALA:H | 2 | 0.76 | 0.35 | 0.76 |
| (3,1139) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 2 | 0.7 | 0.01 | 0.7 |
| (2,46) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HA | 2 | 0.67 | 0.02 | 0.67 |
| (3,354) | 1:115:A:VAL:H | 1:118:A:ILE:HG13 | 2 | 0.67 | 0.04 | 0.67 |
| (3,354) | 1:115:A:VAL:H | 1:114:A:ARG:HG3 | 2 | 0.67 | 0.04 | 0.67 |
| (1,926) | 1:58:A:LYS:HG3 | 1:59:A:LEU:H | 2 | 0.66 | 0.56 | 0.66 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,1156) | 1:10:A:ARG:HG2 | 1:10:A:ARG:H | 2 | 0.66 | 0.3 | 0.66 |
| (3,1156) | 1:9:A:ALA:HB2 | 1:10:A:ARG:H | 2 | 0.66 | 0.3 | 0.66 |
| (1,2784) | 1:82:A:GLY:H | 1:10:A:ARG:HG2 | 2 | 0.6 | 0.22 | 0.6 |
| (1,2536) | 1:106:A:GLU:HG2 | 1:104:A:VAL:H | 2 | 0.58 | 0.01 | 0.58 |
| (1,2584) | 1:100:A:SER:H | 1:119:A:GLN:HE22 | 2 | 0.58 | 0.25 | 0.58 |
| (1,441) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HA | 2 | 0.57 | 0.03 | 0.57 |
| (1,441) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HA | 2 | 0.57 | 0.03 | 0.57 |
| (1,441) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HA | 2 | 0.57 | 0.03 | 0.57 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG21 | 2 | 0.57 | 0.04 | 0.57 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG22 | 2 | 0.57 | 0.04 | 0.57 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG23 | 2 | 0.57 | 0.04 | 0.57 |
| (1,477) | 1:31:A:LYS:HB2 | 1:31:A:LYS:HA | 2 | 0.56 | 0.0 | 0.56 |
| (3,1049) | 1:109:A:PRO:HA | 1:109:A:PRO:HG2 | 2 | 0.54 | 0.01 | 0.54 |
| (3,800) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 2 | 0.52 | 0.02 | 0.52 |
| (1,3522) | 1:40:A:LYS:HE3 | 1:51:A:LYS:H | 2 | 0.52 | 0.1 | 0.52 |
| (3,240) | 1:109:A:PRO:HA | 1:109:A:PRO:HG2 | 2 | 0.52 | 0.01 | 0.52 |
| (1,1481) | 1:88:A:GLU:HG3 | 1:88:A:GLU:H | 2 | 0.51 | 0.04 | 0.51 |
| (3,615) | 1:105:A:ILE:HA | 1:87:A:ASN:HB2 | 2 | 0.51 | 0.34 | 0.51 |
| (3,615) | 1:26:A:LYS:HE3 | 1:30:A:GLU:HA | 2 | 0.51 | 0.34 | 0.51 |
| (1,2708) | 1:88:A:GLU:HB3 | 1:89:A:GLY:H | 2 | 0.5 | 0.01 | 0.5 |
| (1,1478) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HB3 | 2 | 0.48 | 0.1 | 0.48 |
| (1,1478) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HB3 | 2 | 0.48 | 0.1 | 0.48 |
| (1,1478) | 1:126:A:LEU:HD23 | 1:88:A:GLU:HB3 | 2 | 0.48 | 0.1 | 0.48 |
| (2,386) | 1:95:A:ASN:HB2 | 1:99:A:PHE:HA | 2 | 0.48 | 0.28 | 0.48 |
| (1,896) | 1:51:A:LYS:HE2 | 1:56:A:GLY:HA2 | 2 | 0.44 | 0.25 | 0.44 |
| (1,817) | 1:51:A:LYS:HG2 | 1:56:A:GLY:HA3 | 2 | 0.44 | 0.16 | 0.44 |
| (1,817) | 1:51:A:LYS:HG3 | 1:56:A:GLY:HA3 | 2 | 0.44 | 0.16 | 0.44 |
| (3,1095) | 1:26:A:LYS:HB3 | 1:25:A:THR:H | 2 | 0.42 | 0.18 | 0.42 |
| (3,1095) | 1:27:A:LYS:HB3 | 1:25:A:THR:H | 2 | 0.42 | 0.18 | 0.42 |
| (3,174) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 2 | 0.42 | 0.01 | 0.42 |
| (1,3501) | 1:40:A:LYS:HE3 | 1:38:A:ILE:H | 2 | 0.42 | 0.28 | 0.42 |
| (1,18) | 1:97:A:LYS:HG3 | 1:97:A:LYS:HA | 2 | 0.41 | 0.0 | 0.41 |
| (3,1068) | 1:126:A:LEU:H | 1:76:A:ARG:HB2 | 2 | 0.39 | 0.24 | 0.39 |
| (1,1810) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD2 | 2 | 0.38 | 0.01 | 0.38 |
| (1,3777) | 1:45:A:LYS:HG2 | 1:46:A:TYR:HD1 | 2 | 0.38 | 0.06 | 0.38 |
| (1,3777) | 1:45:A:LYS:HG2 | 1:46:A:TYR:HD2 | 2 | 0.38 | 0.06 | 0.38 |
| (3,416) | 1:5:A:LYS:H | 1:4:A:GLU:HG3 | 2 | 0.38 | 0.14 | 0.38 |
| (3,416) | 1:5:A:LYS:H | 1:4:A:GLU:HG2 | 2 | 0.38 | 0.14 | 0.38 |
| (1,2071) | 1:126:A:LEU:HB2 | 1:76:A:ARG:HB3 | 2 | 0.38 | 0.09 | 0.38 |
| (3,475) | 1:32:A:TYR:HB2 | 1:30:A:GLU:HA | 2 | 0.37 | 0.25 | 0.37 |
| (3,475) | 1:26:A:LYS:HE3 | 1:30:A:GLU:HA | 2 | 0.37 | 0.25 | 0.37 |
| (3,1154) | 1:6:A:LYS:HB3 | 1:7:A:ARG:H | 2 | 0.37 | 0.1 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1154) | 1:7:A:ARG:HB2 | 1:7:A:ARG:H | 2 | 0.37 | 0.1 | 0.37 |
| (1,621) | 1:41:A:GLU:HA | 1:41:A:GLU:HG3 | 2 | 0.36 | 0.08 | 0.36 |
| (1,2517) | 1:88:A:GLU:HB2 | 1:106:A:GLU:H | 2 | 0.36 | 0.02 | 0.36 |
| (1,3556) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 2 | 0.36 | 0.16 | 0.36 |
| (3,900) | 1:34:A:LYS:HE3 | 1:34:A:LYS:HG3 | 2 | 0.36 | 0.22 | 0.36 |
| (3,1060) | 1:9:A:ALA:HB3 | 1:9:A:ALA:H | 2 | 0.35 | 0.05 | 0.35 |
| (3,1060) | 1:9:A:ALA:HB2 | 1:9:A:ALA:H | 2 | 0.35 | 0.05 | 0.35 |
| (1,3098) | 1:44:A:ASP:HB2 | 1:47:A:THR:H | 2 | 0.34 | 0.06 | 0.34 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD11 | 2 | 0.34 | 0.0 | 0.34 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD12 | 2 | 0.34 | 0.0 | 0.34 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD13 | 2 | 0.34 | 0.0 | 0.34 |
| (1,1608) | 1:97:A:LYS:HG2 | 1:97:A:LYS:HA | 2 | 0.34 | 0.03 | 0.34 |
| (1,818) | 1:51:A:LYS:HG2 | 1:56:A:GLY:HA3 | 2 | 0.34 | 0.16 | 0.34 |
| (1,818) | 1:51:A:LYS:HG3 | 1:56:A:GLY:HA3 | 2 | 0.34 | 0.16 | 0.34 |
| (1,3443) | 1:63:A:GLN:HG3 | 1:14:A:TRP:HE1 | 2 | 0.34 | 0.23 | 0.34 |
| (1,893) | 1:51:A:LYS:HG2 | 1:56:A:GLY:HA3 | 2 | 0.32 | 0.16 | 0.32 |
| (1,893) | 1:51:A:LYS:HG3 | 1:56:A:GLY:HA3 | 2 | 0.32 | 0.16 | 0.32 |
| (1,3842) | 1:46:A:TYR:HE1 | 1:45:A:LYS:HB2 | 2 | 0.32 | 0.1 | 0.32 |
| (1,3842) | 1:46:A:TYR:HE2 | 1:45:A:LYS:HB2 | 2 | 0.32 | 0.1 | 0.32 |
| (2,520) | 1:78:A:LEU:H | 1:88:A:GLU:HG2 | 2 | 0.32 | 0.05 | 0.32 |
| (1,3015) | 1:32:A:TYR:HE1 | 1:57:A:ASP:H | 2 | 0.31 | 0.16 | 0.31 |
| (1,3015) | 1:32:A:TYR:HE2 | 1:57:A:ASP:H | 2 | 0.31 | 0.16 | 0.31 |
| (3,865) | 1:31:A:LYS:HG2 | 1:31:A:LYS:HE2 | 2 | 0.31 | 0.0 | 0.31 |
| (2,591) | 1:11:A:THR:H | 1:13:A:TYR:HD1 | 2 | 0.3 | 0.04 | 0.3 |
| (2,591) | 1:11:A:THR:H | 1:13:A:TYR:HD2 | 2 | 0.3 | 0.04 | 0.3 |
| (1,3782) | 1:11:A:THR:HB | 1:13:A:TYR:HD1 | 2 | 0.3 | 0.12 | 0.3 |
| (1,3782) | 1:11:A:THR:HB | 1:13:A:TYR:HD2 | 2 | 0.3 | 0.12 | 0.3 |
| (1,3027) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 2 | 0.29 | 0.16 | 0.29 |
| (1,2622) | 1:97:A:LYS:H | 1:97:A:LYS:HG3 | 2 | 0.27 | 0.02 | 0.27 |
| (3,43) | 1:77:A:ILE:H | 1:77:A:ILE:HD13 | 2 | 0.26 | 0.08 | 0.26 |
| (3,43) | 1:77:A:ILE:H | 1:77:A:ILE:HG22 | 2 | 0.26 | 0.08 | 0.26 |
| (1,423) | 1:26:A:LYS:HG3 | 1:26:A:LYS:HE2 | 2 | 0.26 | 0.01 | 0.26 |
| (1,423) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HE3 | 2 | 0.26 | 0.01 | 0.26 |
| (1,1657) | 1:101:A:ALA:HB1 | 1:95:A:ASN:H | 2 | 0.26 | 0.03 | 0.26 |
| (1,1657) | 1:101:A:ALA:HB2 | 1:95:A:ASN:H | 2 | 0.26 | 0.03 | 0.26 |
| (1,1657) | 1:101:A:ALA:HB3 | 1:95:A:ASN:H | 2 | 0.26 | 0.03 | 0.26 |
| (1,2304) | 1:104:A:VAL:HG21 | 1:114:A:ARG:HB3 | 2 | 0.25 | 0.09 | 0.25 |
| (1,2304) | 1:104:A:VAL:HG22 | 1:114:A:ARG:HB3 | 2 | 0.25 | 0.09 | 0.25 |
| (1,2304) | 1:104:A:VAL:HG23 | 1:114:A:ARG:HB3 | 2 | 0.25 | 0.09 | 0.25 |
| (1,2128) | 1:70:A:ILE:HD11 | 1:121:A:GLU:HA | 2 | 0.24 | 0.1 | 0.24 |
| (1,2128) | 1:70:A:ILE:HD12 | 1:121:A:GLU:HA | 2 | 0.24 | 0.1 | 0.24 |
| (1,2128) | 1:70:A:ILE:HD13 | 1:121:A:GLU:HA | 2 | 0.24 | 0.1 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3499) | 1:37:A:ALA:H | 1:36:A:LYS:HE2 | 2 | 0.24 | 0.03 | 0.24 |
| (1,3402) | 1:9:A:ALA:HA | 1:10:A:ARG:H | 2 | 0.23 | 0.1 | 0.23 |
| (1,2271) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HA | 2 | 0.22 | 0.03 | 0.22 |
| (1,2271) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HA | 2 | 0.22 | 0.03 | 0.22 |
| (1,2271) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HA | 2 | 0.22 | 0.03 | 0.22 |
| (1,3759) | 1:27:A:LYS:HG3 | 1:65:A:HIS:HE1 | 2 | 0.22 | 0.02 | 0.22 |
| (1,3415) | 1:7:A:ARG:HG3 | 1:7:A:ARG:H | 2 | 0.22 | 0.1 | 0.22 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG21 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG23 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG21 | 2 | 0.2 | 0.06 | 0.2 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG22 | 2 | 0.2 | 0.06 | 0.2 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG23 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1434) | 1:85:A:ARG:HA | 1:81:A:ASN:HA | 2 | 0.2 | 0.06 | 0.2 |
| (1,2196) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 2 | 0.2 | 0.04 | 0.2 |
| (1,3696) | 1:68:A:THR:H | 1:14:A:TRP:HZ2 | 2 | 0.2 | 0.02 | 0.2 |
| (1,1555) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 2 | 0.19 | 0.03 | 0.19 |
| (1,2843) | 1:105:A:ILE:HG21 | 1:112:A:GLY:H | 2 | 0.19 | 0.01 | 0.19 |
| (1,2843) | 1:105:A:ILE:HG22 | 1:112:A:GLY:H | 2 | 0.19 | 0.01 | 0.19 |
| (1,2843) | 1:105:A:ILE:HG23 | 1:112:A:GLY:H | 2 | 0.19 | 0.01 | 0.19 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG21 | 2 | 0.19 | 0.06 | 0.19 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG22 | 2 | 0.19 | 0.06 | 0.19 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG23 | 2 | 0.19 | 0.06 | 0.19 |
| (3,820) | 1:93:A:SER:H | 1:92:A:GLU:HG2 | 2 | 0.19 | 0.07 | 0.19 |
| (3,820) | 1:117:A:GLY:H | 1:116:A:GLU:HG2 | 2 | 0.19 | 0.07 | 0.19 |
| (3,988) | 1:96:A:GLU:HA | 1:99:A:PHE:H | 2 | 0.18 | 0.02 | 0.18 |
| (1,3389) | 1:82:A:GLY:H | 1:11:A:THR:H | 2 | 0.18 | 0.05 | 0.18 |
| (1,3397) | 1:10:A:ARG:HB3 | 1:11:A:THR:H | 2 | 0.18 | 0.02 | 0.18 |
| (3,721) | 1:51:A:LYS:HG3 | 1:57:A:ASP:HA | 2 | 0.18 | 0.07 | 0.18 |
| (1,1426) | 1:85:A:ARG:HA | 1:87:A:ASN:H | 2 | 0.18 | 0.06 | 0.18 |
| (1,3635) | 1:64:A:THR:H | 1:62:A:ASP:H | 2 | 0.18 | 0.08 | 0.18 |
| (3,644) | 1:3:A:GLU:HA | 1:4:A:GLU:H | 2 | 0.18 | 0.0 | 0.18 |
| (3,1226) | 1:93:A:SER:H | 1:92:A:GLU:HG2 | 2 | 0.18 | 0.08 | 0.18 |
| (3,1226) | 1:117:A:GLY:H | 1:116:A:GLU:HG2 | 2 | 0.18 | 0.08 | 0.18 |
| (1,2459) | 1:113:A:ARG:H | 1:107:A:THR:H | 2 | 0.17 | 0.03 | 0.17 |
| (1,574) | 1:39:A:VAL:HG11 | 1:40:A:LYS:H | 2 | 0.17 | 0.04 | 0.17 |
| (1,574) | 1:39:A:VAL:HG12 | 1:40:A:LYS:H | 2 | 0.17 | 0.04 | 0.17 |
| (1,574) | 1:39:A:VAL:HG13 | 1:40:A:LYS:H | 2 | 0.17 | 0.04 | 0.17 |
| (1,3028) | 1:51:A:LYS:HG2 | 1:56:A:GLY:H | 2 | 0.17 | 0.05 | 0.17 |
| (1,70) | 1:11:A:THR:HA | 1:11:A:THR:HB | 2 | 0.16 | 0.01 | 0.16 |
| (1,1301) | 1:125:A:LYS:HA | 1:77:A:ILE:HB | 2 | 0.16 | 0.04 | 0.16 |
| (3,1034) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 2 | 0.16 | 0.01 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2102) | 1:126:A:LEU:HD21 | 1:77:A:ILE:H | 2 | 0.16 | 0.05 | 0.16 |
| (1,2102) | 1:126:A:LEU:HD22 | 1:77:A:ILE:H | 2 | 0.16 | 0.05 | 0.16 |
| (1,2102) | 1:126:A:LEU:HD23 | 1:77:A:ILE:H | 2 | 0.16 | 0.05 | 0.16 |
| (2,361) | 1:84:A:TYR:HB2 | 1:103:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,2573) | 1:101:A:ALA:H | 1:100:A:SER:HB2 | 2 | 0.16 | 0.05 | 0.16 |
| (1,3255) | 1:31:A:LYS:HG3 | 1:32:A:TYR:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,2411) | 1:118:A:ILE:H | 1:101:A:ALA:HA | 2 | 0.15 | 0.01 | 0.15 |
| (3,167) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 2 | 0.15 | 0.04 | 0.15 |
| (3,167) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 2 | 0.15 | 0.04 | 0.15 |
| (1,24) | 1:7:A:ARG:HA | 1:7:A:ARG:HB3 | 2 | 0.14 | 0.0 | 0.14 |
| (1,455) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,455) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,455) | 1:28:A:LEU:HD13 | 1:28:A:LEU:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (2,407) | 1:42:A:VAL:HG11 | 1:44:A:ASP:HA | 2 | 0.14 | 0.02 | 0.14 |
| (2,407) | 1:42:A:VAL:HG12 | 1:44:A:ASP:HA | 2 | 0.14 | 0.02 | 0.14 |
| (2,407) | 1:42:A:VAL:HG13 | 1:44:A:ASP:HA | 2 | 0.14 | 0.02 | 0.14 |
| (3,965) | 1:95:A:ASN:H | 1:101:A:ALA:H | 2 | 0.14 | 0.01 | 0.14 |
| (1,1667) | 1:102:A:THR:HA | 1:116:A:GLU:HG2 | 2 | 0.13 | 0.03 | 0.13 |
| (1,2750) | 1:79:A:VAL:HG21 | 1:86:A:GLY:H | 2 | 0.13 | 0.01 | 0.13 |
| (1,2750) | 1:79:A:VAL:HG22 | 1:86:A:GLY:H | 2 | 0.13 | 0.01 | 0.13 |
| (1,2750) | 1:79:A:VAL:HG23 | 1:86:A:GLY:H | 2 | 0.13 | 0.01 | 0.13 |
| (3,552) | 1:32:A:TYR:HE1 | 1:57:A:ASP:HB3 | 2 | 0.13 | 0.02 | 0.13 |
| (3,580) | 1:92:A:GLU:HB3 | 1:92:A:GLU:HA | 2 | 0.13 | 0.0 | 0.13 |
| (3,867) | 1:17:A:PRO:HB3 | 1:18:A:GLU:H | 2 | 0.13 | 0.02 | 0.13 |
| (1,2400) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,3100) | 1:48:A:ALA:HB1 | 1:47:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,3100) | 1:48:A:ALA:HB2 | 1:47:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,3100) | 1:48:A:ALA:HB3 | 1:47:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (3,826) | 1:5:A:LYS:H | 1:5:A:LYS:HA | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG11 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG12 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG13 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG11 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG12 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG13 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG11 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG12 | 2 | 0.12 | 0.02 | 0.12 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG13 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1829) | 1:110:A:LEU:HA | 1:111:A:LYS:H | 2 | 0.12 | 0.0 | 0.12 |
| (3,224) | 1:103:A:ILE:HG21 | 1:101:A:ALA:H | 2 | 0.12 | 0.0 | 0.12 |
| (3,224) | 1:103:A:ILE:HG22 | 1:101:A:ALA:H | 2 | 0.12 | 0.0 | 0.12 |
| (3,1053) | 1:21:A:VAL:HG23 | 1:66:A:LEU:HD21 | 2 | 0.12 | 0.01 | 0.12 |

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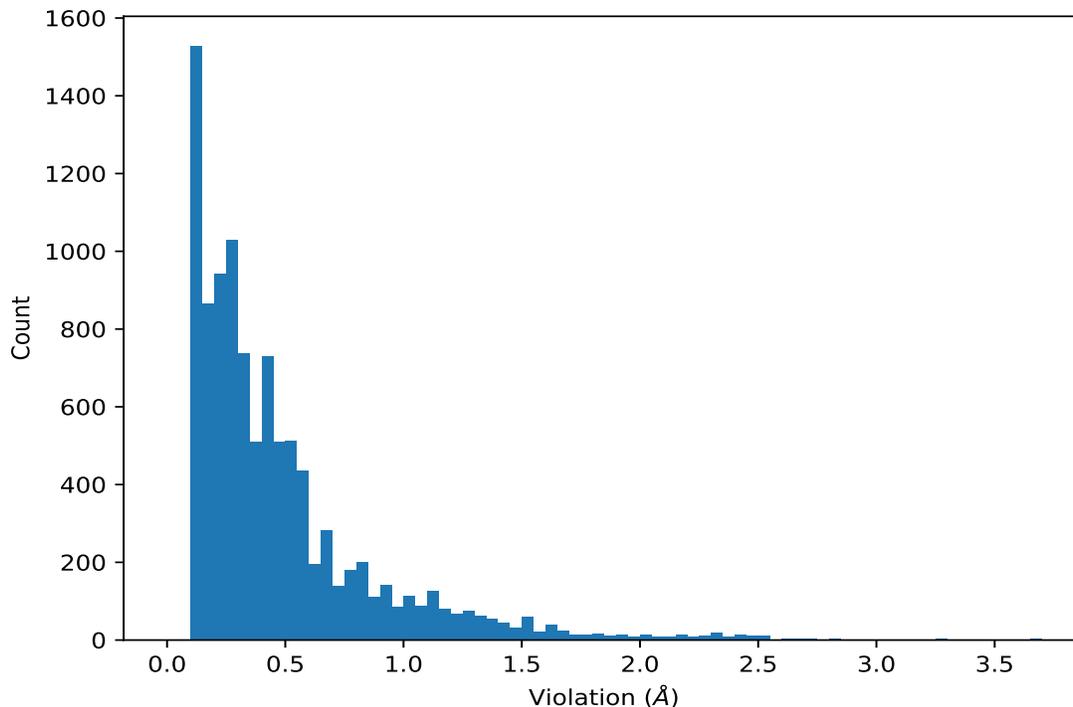
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,1053) | 1:21:A:VAL:HG23 | 1:66:A:LEU:HD22 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3225) | 1:35:A:LYS:H | 1:34:A:LYS:HG3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,747) | 1:46:A:TYR:HA | 1:46:A:TYR:HD1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,747) | 1:46:A:TYR:HA | 1:46:A:TYR:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,374) | 1:23:A:ILE:HG21 | 1:33:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,374) | 1:23:A:ILE:HG22 | 1:33:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,374) | 1:23:A:ILE:HG23 | 1:33:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2607) | 1:97:A:LYS:HG2 | 1:98:A:THR:H | 2 | 0.11 | 0.01 | 0.11 |
| (3,29) | 1:108:A:GLY:H | 1:108:A:GLY:HA3 | 2 | 0.11 | 0.0 | 0.11 |
| (3,915) | 1:76:A:ARG:H | 1:76:A:ARG:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2149) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 2 | 0.11 | 0.0 | 0.11 |
| (3,792) | 1:126:A:LEU:HG | 1:126:A:LEU:HD21 | 2 | 0.11 | 0.0 | 0.11 |
| (3,899) | 1:35:A:LYS:HA | 1:35:A:LYS:H | 2 | 0.11 | 0.0 | 0.11 |
| (3,1153) | 1:3:A:GLU:HA | 1:4:A:GLU:H | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 10 | 3.7 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 10 | 3.7 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 10 | 3.7 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG21 | 10 | 3.27 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG22 | 10 | 3.27 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG23 | 10 | 3.27 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 6 | 3.24 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 5 | 2.97 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 3 | 2.88 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 2 | 2.83 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 2 | 2.83 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 2 | 2.83 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 5 | 2.74 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 9 | 2.72 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 9 | 2.72 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 9 | 2.72 |
| (3,804) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG22 | 10 | 2.7 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 4 | 2.69 |
| (1,2882) | 1:91:A:LEU:HD11 | 1:72:A:ALA:H | 10 | 2.68 |
| (1,2882) | 1:91:A:LEU:HD12 | 1:72:A:ALA:H | 10 | 2.68 |
| (1,2882) | 1:91:A:LEU:HD13 | 1:72:A:ALA:H | 10 | 2.68 |
| (1,2139) | 1:121:A:GLU:HG2 | 1:119:A:GLN:HG3 | 3 | 2.68 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 8 | 2.65 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 8 | 2.65 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 8 | 2.65 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 10 | 2.64 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 8 | 2.59 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 8 | 2.53 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 8 | 2.53 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 8 | 2.53 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 6 | 2.53 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 6 | 2.53 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 6 | 2.53 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 9 | 2.52 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 7 | 2.52 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 3 | 2.52 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 3 | 2.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 3 | 2.52 |
| (1,861) | 1:53:A:ILE:HD11 | 1:36:A:LYS:HE3 | 6 | 2.49 |
| (1,861) | 1:53:A:ILE:HD12 | 1:36:A:LYS:HE3 | 6 | 2.49 |
| (1,861) | 1:53:A:ILE:HD13 | 1:36:A:LYS:HE3 | 6 | 2.49 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 9 | 2.49 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 6 | 2.47 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 4 | 2.45 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 4 | 2.45 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 4 | 2.45 |
| (1,1211) | 1:91:A:LEU:HD11 | 1:72:A:ALA:HA | 10 | 2.45 |
| (1,1211) | 1:91:A:LEU:HD12 | 1:72:A:ALA:HA | 10 | 2.45 |
| (1,1211) | 1:91:A:LEU:HD13 | 1:72:A:ALA:HA | 10 | 2.45 |
| (1,2096) | 1:125:A:LYS:HE2 | 1:127:A:ALA:HA | 1 | 2.43 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 10 | 2.43 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 9 | 2.42 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 9 | 2.42 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 9 | 2.42 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 10 | 2.42 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 10 | 2.42 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 10 | 2.42 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 6 | 2.42 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 9 | 2.42 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 9 | 2.42 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 9 | 2.42 |
| (1,3557) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HD21 | 2 | 2.41 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 10 | 2.4 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 7 | 2.38 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 8 | 2.37 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 9 | 2.37 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 9 | 2.37 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 9 | 2.37 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 10 | 2.35 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 10 | 2.35 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 10 | 2.35 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 8 | 2.34 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 8 | 2.34 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 8 | 2.34 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 7 | 2.34 |
| (3,250) | 1:15:A:LEU:HD12 | 1:66:A:LEU:HD22 | 8 | 2.33 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 2 | 2.33 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 2 | 2.33 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 2 | 2.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,250) | 1:15:A:LEU:HD11 | 1:66:A:LEU:HD23 | 3 | 2.31 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 6 | 2.31 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 6 | 2.31 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 6 | 2.31 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 10 | 2.31 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 10 | 2.31 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 10 | 2.31 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 3 | 2.31 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 8 | 2.31 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 8 | 2.31 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 8 | 2.31 |
| (3,250) | 1:15:A:LEU:HD11 | 1:66:A:LEU:HD22 | 1 | 2.3 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 1 | 2.3 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 5 | 2.3 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 7 | 2.29 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 10 | 2.28 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 10 | 2.28 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 10 | 2.28 |
| (1,3598) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD22 | 5 | 2.27 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 4 | 2.26 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 4 | 2.26 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 4 | 2.26 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD23 | 7 | 2.24 |
| (3,525) | 1:71:A:PRO:HD3 | 1:77:A:ILE:HG22 | 10 | 2.23 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD23 | 5 | 2.22 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 8 | 2.22 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 4 | 2.22 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 5 | 2.21 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 5 | 2.21 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 5 | 2.21 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 10 | 2.19 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 10 | 2.19 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 10 | 2.19 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 9 | 2.17 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD23 | 10 | 2.16 |
| (1,1329) | 1:78:A:LEU:HD21 | 1:79:A:VAL:H | 6 | 2.16 |
| (1,1329) | 1:78:A:LEU:HD22 | 1:79:A:VAL:H | 6 | 2.16 |
| (1,1329) | 1:78:A:LEU:HD23 | 1:79:A:VAL:H | 6 | 2.16 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 8 | 2.16 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 1 | 2.16 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 1 | 2.16 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 1 | 2.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,250) | 1:15:A:LEU:HD12 | 1:66:A:LEU:HD23 | 4 | 2.15 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 2 | 2.15 |
| (3,250) | 1:15:A:LEU:HD12 | 1:66:A:LEU:HD21 | 2 | 2.13 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 10 | 2.13 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 6 | 2.13 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 6 | 2.13 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 6 | 2.13 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD23 | 6 | 2.12 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 3 | 2.12 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 9 | 2.11 |
| (3,250) | 1:15:A:LEU:HD13 | 1:66:A:LEU:HD21 | 9 | 2.09 |
| (1,2097) | 1:18:A:GLU:HG3 | 1:127:A:ALA:HA | 7 | 2.09 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 3 | 2.09 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 1 | 2.08 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 1 | 2.08 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 1 | 2.08 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 10 | 2.07 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 1 | 2.07 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 3 | 2.05 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 3 | 2.05 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 3 | 2.05 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 4 | 2.05 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 2 | 2.05 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 5 | 2.05 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 5 | 2.05 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 5 | 2.05 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 7 | 2.04 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 10 | 2.02 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 5 | 2.02 |
| (1,963) | 1:34:A:LYS:HE2 | 1:33:A:HIS:HE1 | 1 | 2.02 |
| (1,1349) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HD22 | 10 | 2.01 |
| (1,1349) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HD22 | 10 | 2.01 |
| (1,1349) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HD22 | 10 | 2.01 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 7 | 1.99 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 7 | 1.99 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 7 | 1.99 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 10 | 1.98 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 10 | 1.98 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 10 | 1.98 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 9 | 1.98 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG11 | 9 | 1.96 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG12 | 9 | 1.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG13 | 9 | 1.96 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 4 | 1.95 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 10 | 1.94 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 10 | 1.94 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 10 | 1.94 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG11 | 10 | 1.93 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG12 | 10 | 1.93 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG13 | 10 | 1.93 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 1 | 1.93 |
| (1,3755) | 1:34:A:LYS:HE2 | 1:33:A:HIS:HE1 | 1 | 1.92 |
| (1,1378) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HD22 | 10 | 1.91 |
| (1,1378) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HD22 | 10 | 1.91 |
| (1,1378) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HD22 | 10 | 1.91 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 6 | 1.91 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 8 | 1.91 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG11 | 4 | 1.89 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG12 | 4 | 1.89 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG13 | 4 | 1.89 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 2 | 1.88 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG11 | 8 | 1.86 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG12 | 8 | 1.86 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG13 | 8 | 1.86 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 9 | 1.85 |
| (1,3758) | 1:65:A:HIS:HE1 | 1:27:A:LYS:HD2 | 9 | 1.85 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 9 | 1.85 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 8 | 1.85 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG11 | 6 | 1.84 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG12 | 6 | 1.84 |
| (1,1920) | 1:104:A:VAL:HA | 1:115:A:VAL:HG13 | 6 | 1.84 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 3 | 1.84 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 3 | 1.84 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 3 | 1.84 |
| (1,425) | 1:91:A:LEU:HD21 | 1:92:A:GLU:H | 10 | 1.83 |
| (1,425) | 1:91:A:LEU:HD22 | 1:92:A:GLU:H | 10 | 1.83 |
| (1,425) | 1:91:A:LEU:HD23 | 1:92:A:GLU:H | 10 | 1.83 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 10 | 1.82 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 4 | 1.82 |
| (1,394) | 1:24:A:ILE:HG12 | 1:67:A:GLU:HB3 | 5 | 1.81 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 4 | 1.81 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 9 | 1.8 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 9 | 1.8 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 9 | 1.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,471) | 1:26:A:LYS:HG3 | 1:30:A:GLU:HA | 10 | 1.8 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 8 | 1.79 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 8 | 1.79 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 8 | 1.79 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 10 | 1.78 |
| (1,861) | 1:53:A:ILE:HD11 | 1:36:A:LYS:HE2 | 3 | 1.78 |
| (1,861) | 1:53:A:ILE:HD12 | 1:36:A:LYS:HE2 | 3 | 1.78 |
| (1,861) | 1:53:A:ILE:HD13 | 1:36:A:LYS:HE2 | 3 | 1.78 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 6 | 1.77 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 6 | 1.77 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 6 | 1.77 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 7 | 1.76 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 6 | 1.75 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 8 | 1.75 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 5 | 1.74 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 5 | 1.74 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 5 | 1.74 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 5 | 1.73 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 9 | 1.72 |
| (1,426) | 1:91:A:LEU:HD21 | 1:102:A:THR:H | 10 | 1.72 |
| (1,426) | 1:91:A:LEU:HD22 | 1:102:A:THR:H | 10 | 1.72 |
| (1,426) | 1:91:A:LEU:HD23 | 1:102:A:THR:H | 10 | 1.72 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 10 | 1.71 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 7 | 1.71 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 7 | 1.71 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 7 | 1.71 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 7 | 1.71 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 7 | 1.71 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 7 | 1.71 |
| (1,3421) | 1:10:A:ARG:H | 1:82:A:GLY:HA3 | 3 | 1.69 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 5 | 1.69 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 3 | 1.69 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 3 | 1.69 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 3 | 1.69 |
| (1,157) | 1:16:A:GLN:HB2 | 1:78:A:LEU:HD11 | 6 | 1.69 |
| (1,157) | 1:16:A:GLN:HB2 | 1:78:A:LEU:HD12 | 6 | 1.69 |
| (1,157) | 1:16:A:GLN:HB2 | 1:78:A:LEU:HD13 | 6 | 1.69 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 1 | 1.68 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 1 | 1.68 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 1 | 1.68 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 4 | 1.68 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 4 | 1.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 4 | 1.68 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 6 | 1.67 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 9 | 1.67 |
| (1,1111) | 1:22:A:LYS:HB2 | 1:67:A:GLU:HB2 | 5 | 1.67 |
| (1,861) | 1:53:A:ILE:HD11 | 1:36:A:LYS:HE2 | 5 | 1.67 |
| (1,861) | 1:53:A:ILE:HD12 | 1:36:A:LYS:HE2 | 5 | 1.67 |
| (1,861) | 1:53:A:ILE:HD13 | 1:36:A:LYS:HE2 | 5 | 1.67 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 10 | 1.66 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 10 | 1.66 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 10 | 1.66 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 5 | 1.66 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 7 | 1.65 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 8 | 1.65 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 8 | 1.65 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 8 | 1.65 |
| (1,1843) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HD22 | 10 | 1.64 |
| (1,1843) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HD22 | 10 | 1.64 |
| (1,1843) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HD22 | 10 | 1.64 |
| (3,555) | 1:12:A:ASP:HB2 | 1:46:A:TYR:HE2 | 10 | 1.63 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 3 | 1.63 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 3 | 1.63 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 4 | 1.63 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 6 | 1.63 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 9 | 1.63 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 9 | 1.63 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 9 | 1.63 |
| (3,186) | 1:59:A:LEU:H | 1:57:A:ASP:HB2 | 6 | 1.62 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 3 | 1.62 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 7 | 1.62 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 1 | 1.62 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 10 | 1.62 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 10 | 1.62 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 10 | 1.62 |
| (1,2821) | 1:78:A:LEU:HD21 | 1:79:A:VAL:H | 6 | 1.61 |
| (1,2821) | 1:78:A:LEU:HD22 | 1:79:A:VAL:H | 6 | 1.61 |
| (1,2821) | 1:78:A:LEU:HD23 | 1:79:A:VAL:H | 6 | 1.61 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 2 | 1.61 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 4 | 1.61 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 4 | 1.61 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 4 | 1.61 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 4 | 1.61 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 10 | 1.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,232) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HA | 10 | 1.6 |
| (2,232) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HA | 10 | 1.6 |
| (2,232) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HA | 10 | 1.6 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 9 | 1.6 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 5 | 1.6 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 4 | 1.6 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 4 | 1.6 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 4 | 1.6 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 6 | 1.59 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 8 | 1.59 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 10 | 1.59 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 6 | 1.58 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 6 | 1.58 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 6 | 1.58 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 6 | 1.58 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 10 | 1.58 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 10 | 1.58 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 10 | 1.58 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 2 | 1.58 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 2 | 1.58 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 2 | 1.58 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 9 | 1.57 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 4 | 1.57 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 7 | 1.57 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 7 | 1.57 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 7 | 1.57 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 2 | 1.56 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 2 | 1.56 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 2 | 1.56 |
| (1,1258) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 10 | 1.55 |
| (3,961) | 1:30:A:GLU:HG2 | 1:29:A:GLY:H | 7 | 1.54 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 7 | 1.54 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 10 | 1.54 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 4 | 1.54 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD11 | 9 | 1.53 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 1 | 1.53 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 5 | 1.53 |
| (1,2677) | 1:91:A:LEU:HD21 | 1:92:A:GLU:H | 10 | 1.53 |
| (1,2677) | 1:91:A:LEU:HD22 | 1:92:A:GLU:H | 10 | 1.53 |
| (1,2677) | 1:91:A:LEU:HD23 | 1:92:A:GLU:H | 10 | 1.53 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 5 | 1.53 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 4 | 1.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 4 | 1.53 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 4 | 1.53 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 6 | 1.53 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 6 | 1.53 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 6 | 1.53 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 7 | 1.52 |
| (1,1926) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 9 | 1.52 |
| (1,1926) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 9 | 1.52 |
| (1,1926) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 9 | 1.52 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 7 | 1.52 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 7 | 1.52 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 7 | 1.52 |
| (1,1262) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 10 | 1.52 |
| (1,834) | 1:52:A:MET:HG2 | 1:59:A:LEU:HG | 6 | 1.52 |
| (1,62) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HB3 | 6 | 1.52 |
| (1,62) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HB3 | 6 | 1.52 |
| (1,62) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HB3 | 6 | 1.52 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 4 | 1.51 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 7 | 1.51 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 6 | 1.51 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 4 | 1.51 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 5 | 1.51 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 7 | 1.51 |
| (1,1926) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 8 | 1.51 |
| (1,1926) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 8 | 1.51 |
| (1,1926) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 8 | 1.51 |
| (1,1353) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HB2 | 10 | 1.51 |
| (1,1353) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HB2 | 10 | 1.51 |
| (1,1353) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HB2 | 10 | 1.51 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 9 | 1.51 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 9 | 1.51 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 9 | 1.51 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 8 | 1.5 |
| (1,2221) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HA | 10 | 1.5 |
| (1,2221) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HA | 10 | 1.5 |
| (1,2221) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 10 | 1.5 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 1 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 5 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 5 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 5 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 9 | 1.5 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 9 | 1.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 9 | 1.5 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 8 | 1.5 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 8 | 1.5 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 8 | 1.5 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 2 | 1.5 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 3 | 1.5 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 5 | 1.49 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 4 | 1.49 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 4 | 1.49 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 4 | 1.49 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 4 | 1.48 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 5 | 1.48 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 5 | 1.48 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 5 | 1.48 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 5 | 1.48 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 3 | 1.48 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 3 | 1.48 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 3 | 1.48 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 1 | 1.48 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 9 | 1.48 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 9 | 1.48 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 9 | 1.48 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD11 | 8 | 1.47 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 3 | 1.47 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 2 | 1.47 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 3 | 1.47 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 3 | 1.47 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 8 | 1.47 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 8 | 1.47 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 8 | 1.47 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 6 | 1.47 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 6 | 1.47 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 1 | 1.47 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 7 | 1.47 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 7 | 1.47 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 7 | 1.47 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 10 | 1.46 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 3 | 1.46 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 10 | 1.45 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 6 | 1.45 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 1 | 1.45 |
| (1,2107) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HB3 | 4 | 1.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2107) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HB3 | 4 | 1.45 |
| (1,2107) | 1:126:A:LEU:HD23 | 1:88:A:GLU:HB3 | 4 | 1.45 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 6 | 1.45 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 6 | 1.45 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 6 | 1.45 |
| (1,1197) | 1:75:A:LYS:HE3 | 1:71:A:PRO:HB2 | 4 | 1.45 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 3 | 1.45 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 3 | 1.45 |
| (3,186) | 1:59:A:LEU:H | 1:57:A:ASP:HB2 | 5 | 1.44 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 2 | 1.44 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 7 | 1.44 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 5 | 1.44 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 10 | 1.44 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 1 | 1.44 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 1 | 1.44 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 1 | 1.44 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 10 | 1.44 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 10 | 1.44 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 10 | 1.44 |
| (1,14) | 1:5:A:LYS:HA | 1:5:A:LYS:HD2 | 2 | 1.44 |
| (3,317) | 1:34:A:LYS:HB2 | 1:34:A:LYS:HE2 | 3 | 1.43 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 8 | 1.43 |
| (1,2039) | 1:110:A:LEU:HD21 | 1:84:A:TYR:HA | 10 | 1.43 |
| (1,2039) | 1:110:A:LEU:HD22 | 1:84:A:TYR:HA | 10 | 1.43 |
| (1,2039) | 1:110:A:LEU:HD23 | 1:84:A:TYR:HA | 10 | 1.43 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 8 | 1.43 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 8 | 1.43 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 8 | 1.43 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 7 | 1.43 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 5 | 1.42 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 3 | 1.42 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 10 | 1.42 |
| (1,1898) | 1:115:A:VAL:H | 1:114:A:ARG:HG2 | 7 | 1.42 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 10 | 1.42 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 10 | 1.42 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 10 | 1.42 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 2 | 1.42 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD13 | 6 | 1.41 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 6 | 1.41 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 6 | 1.41 |
| (3,518) | 1:96:A:GLU:HG3 | 1:97:A:LYS:HG3 | 8 | 1.4 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 5 | 1.4 |

Continued on next page...

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD11 | 4 | 1.39 |
| (3,501) | 1:49:A:VAL:HG12 | 1:40:A:LYS:HB3 | 4 | 1.39 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 2 | 1.39 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 10 | 1.39 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 3 | 1.39 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 10 | 1.39 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 7 | 1.39 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 1 | 1.39 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 2 | 1.39 |
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 2 | 1.39 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 2 | 1.39 |
| (1,769) | 1:42:A:VAL:HG21 | 1:48:A:ALA:HA | 5 | 1.39 |
| (1,769) | 1:42:A:VAL:HG22 | 1:48:A:ALA:HA | 5 | 1.39 |
| (1,769) | 1:42:A:VAL:HG23 | 1:48:A:ALA:HA | 5 | 1.39 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 6 | 1.38 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 7 | 1.38 |
| (1,1926) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 10 | 1.38 |
| (1,1926) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 10 | 1.38 |
| (1,1926) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 10 | 1.38 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 9 | 1.38 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 7 | 1.38 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 7 | 1.38 |
| (1,170) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HG3 | 6 | 1.38 |
| (1,170) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HG3 | 6 | 1.38 |
| (1,170) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HG3 | 6 | 1.38 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD13 | 10 | 1.37 |
| (3,31) | 1:75:A:LYS:HE2 | 1:76:A:ARG:H | 3 | 1.37 |
| (1,3563) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HD21 | 10 | 1.37 |
| (1,3563) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HD21 | 10 | 1.37 |
| (1,3563) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HD21 | 10 | 1.37 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 6 | 1.37 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 3 | 1.37 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 8 | 1.37 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 4 | 1.37 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 5 | 1.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3421) | 1:10:A:ARG:H | 1:82:A:GLY:HA3 | 1 | 1.36 |
| (3,317) | 1:34:A:LYS:HB3 | 1:34:A:LYS:HE2 | 10 | 1.35 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 6 | 1.35 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 5 | 1.35 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 5 | 1.35 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 5 | 1.35 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 2 | 1.35 |
| (1,427) | 1:91:A:LEU:HD21 | 1:93:A:SER:H | 10 | 1.35 |
| (1,427) | 1:91:A:LEU:HD22 | 1:93:A:SER:H | 10 | 1.35 |
| (1,427) | 1:91:A:LEU:HD23 | 1:93:A:SER:H | 10 | 1.35 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 4 | 1.34 |
| (1,23) | 1:7:A:ARG:HA | 1:7:A:ARG:HD3 | 1 | 1.34 |
| (3,501) | 1:49:A:VAL:HG12 | 1:40:A:LYS:HB3 | 10 | 1.33 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 5 | 1.33 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 7 | 1.33 |
| (1,2502) | 1:107:A:THR:H | 1:87:A:ASN:HB2 | 3 | 1.33 |
| (1,2420) | 1:115:A:VAL:HG21 | 1:118:A:ILE:H | 4 | 1.33 |
| (1,2420) | 1:115:A:VAL:HG22 | 1:118:A:ILE:H | 4 | 1.33 |
| (1,2420) | 1:115:A:VAL:HG23 | 1:118:A:ILE:H | 4 | 1.33 |
| (1,2420) | 1:115:A:VAL:HG21 | 1:118:A:ILE:H | 9 | 1.33 |
| (1,2420) | 1:115:A:VAL:HG22 | 1:118:A:ILE:H | 9 | 1.33 |
| (1,2420) | 1:115:A:VAL:HG23 | 1:118:A:ILE:H | 9 | 1.33 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 6 | 1.33 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 6 | 1.33 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 6 | 1.33 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 3 | 1.33 |
| (1,452) | 1:28:A:LEU:HD11 | 1:60:A:LYS:H | 9 | 1.33 |
| (1,452) | 1:28:A:LEU:HD12 | 1:60:A:LYS:H | 9 | 1.33 |
| (1,452) | 1:28:A:LEU:HD13 | 1:60:A:LYS:H | 9 | 1.33 |
| (3,31) | 1:75:A:LYS:HE3 | 1:76:A:ARG:H | 7 | 1.32 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 2 | 1.32 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 9 | 1.32 |
| (1,2106) | 1:109:A:PRO:HB2 | 1:110:A:LEU:HD11 | 10 | 1.32 |
| (1,2106) | 1:109:A:PRO:HB2 | 1:110:A:LEU:HD12 | 10 | 1.32 |
| (1,2106) | 1:109:A:PRO:HB2 | 1:110:A:LEU:HD13 | 10 | 1.32 |
| (1,1926) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 4 | 1.32 |
| (1,1926) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 4 | 1.32 |
| (1,1926) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 4 | 1.32 |
| (1,1884) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HD3 | 2 | 1.32 |
| (1,1884) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HD3 | 2 | 1.32 |
| (1,1884) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HD3 | 2 | 1.32 |
| (1,1723) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 1 | 1.32 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1723) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 1 | 1.32 |
| (1,1723) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 1 | 1.32 |
| (1,834) | 1:52:A:MET:HG2 | 1:59:A:LEU:HG | 7 | 1.32 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 5 | 1.32 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 5 | 1.32 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 5 | 1.32 |
| (3,735) | 1:115:A:VAL:HG13 | 1:103:A:ILE:HD13 | 10 | 1.31 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 8 | 1.31 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 4 | 1.31 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 9 | 1.31 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 1 | 1.31 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 5 | 1.31 |
| (1,2432) | 1:115:A:VAL:HG21 | 1:116:A:GLU:H | 10 | 1.31 |
| (1,2432) | 1:115:A:VAL:HG22 | 1:116:A:GLU:H | 10 | 1.31 |
| (1,2432) | 1:115:A:VAL:HG23 | 1:116:A:GLU:H | 10 | 1.31 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 1 | 1.3 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 1 | 1.3 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 10 | 1.3 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 1 | 1.3 |
| (1,2533) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 9 | 1.3 |
| (1,2533) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 9 | 1.3 |
| (1,2533) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 9 | 1.3 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 6 | 1.3 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 6 | 1.3 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 6 | 1.3 |
| (1,1921) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 10 | 1.3 |
| (1,1921) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 10 | 1.3 |
| (1,1921) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 10 | 1.3 |
| (1,604) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HA | 10 | 1.3 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 6 | 1.3 |
| (3,814) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 7 | 1.29 |
| (3,317) | 1:34:A:LYS:HB3 | 1:34:A:LYS:HE2 | 2 | 1.29 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 1 | 1.29 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 6 | 1.29 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 4 | 1.29 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 4 | 1.29 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 4 | 1.29 |
| (1,2103) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 2 | 1.29 |
| (3,1179) | 1:27:A:LYS:HA | 1:27:A:LYS:HD2 | 3 | 1.28 |
| (3,1097) | 1:82:A:GLY:H | 1:79:A:VAL:HG21 | 3 | 1.28 |
| (3,317) | 1:34:A:LYS:HB3 | 1:34:A:LYS:HE2 | 8 | 1.28 |
| (2,344) | 1:81:A:ASN:HB3 | 1:123:A:ILE:HA | 9 | 1.28 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 7 | 1.28 |
| (1,2533) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 10 | 1.28 |
| (1,2533) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 10 | 1.28 |
| (1,2533) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 10 | 1.28 |
| (1,2420) | 1:115:A:VAL:HG21 | 1:118:A:ILE:H | 10 | 1.28 |
| (1,2420) | 1:115:A:VAL:HG22 | 1:118:A:ILE:H | 10 | 1.28 |
| (1,2420) | 1:115:A:VAL:HG23 | 1:118:A:ILE:H | 10 | 1.28 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 7 | 1.28 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 1 | 1.28 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 1 | 1.28 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 1 | 1.28 |
| (1,1790) | 1:107:A:THR:HG21 | 1:88:A:GLU:HG3 | 1 | 1.28 |
| (1,1790) | 1:107:A:THR:HG22 | 1:88:A:GLU:HG3 | 1 | 1.28 |
| (1,1790) | 1:107:A:THR:HG23 | 1:88:A:GLU:HG3 | 1 | 1.28 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG21 | 5 | 1.28 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG22 | 5 | 1.28 |
| (1,664) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG23 | 5 | 1.28 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 6 | 1.28 |
| (1,428) | 1:91:A:LEU:HD21 | 1:91:A:LEU:HA | 10 | 1.28 |
| (1,428) | 1:91:A:LEU:HD22 | 1:91:A:LEU:HA | 10 | 1.28 |
| (1,428) | 1:91:A:LEU:HD23 | 1:91:A:LEU:HA | 10 | 1.28 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 10 | 1.27 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 2 | 1.27 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 8 | 1.27 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 2 | 1.27 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 2 | 1.27 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 2 | 1.27 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 7 | 1.27 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 7 | 1.27 |
| (1,23) | 1:7:A:ARG:HA | 1:7:A:ARG:HD3 | 6 | 1.27 |
| (1,3453) | 1:14:A:TRP:HA | 1:16:A:GLN:HE22 | 10 | 1.26 |
| (1,2533) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 8 | 1.26 |
| (1,2533) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 8 | 1.26 |
| (1,2533) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 8 | 1.26 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 4 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2239) | 1:10:A:ARG:HG2 | 1:82:A:GLY:HA3 | 2 | 1.26 |
| (1,1921) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 8 | 1.26 |
| (1,1921) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 8 | 1.26 |
| (1,1921) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 8 | 1.26 |
| (1,963) | 1:34:A:LYS:HE2 | 1:33:A:HIS:HE1 | 7 | 1.26 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 4 | 1.26 |
| (1,48) | 1:3:A:GLU:HB2 | 1:8:A:THR:HB | 1 | 1.26 |
| (3,241) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HE22 | 2 | 1.25 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 8 | 1.25 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 1 | 1.25 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 6 | 1.25 |
| (1,2697) | 1:106:A:GLU:HG2 | 1:90:A:THR:H | 6 | 1.25 |
| (1,2667) | 1:91:A:LEU:HD21 | 1:93:A:SER:H | 10 | 1.25 |
| (1,2667) | 1:91:A:LEU:HD22 | 1:93:A:SER:H | 10 | 1.25 |
| (1,2667) | 1:91:A:LEU:HD23 | 1:93:A:SER:H | 10 | 1.25 |
| (1,2107) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HB3 | 1 | 1.25 |
| (1,2107) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HB3 | 1 | 1.25 |
| (1,2107) | 1:126:A:LEU:HD23 | 1:88:A:GLU:HB3 | 1 | 1.25 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 6 | 1.25 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 7 | 1.25 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 7 | 1.25 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 3 | 1.25 |
| (3,1179) | 1:27:A:LYS:HA | 1:27:A:LYS:HD2 | 10 | 1.24 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 4 | 1.24 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 4 | 1.24 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 4 | 1.24 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 6 | 1.24 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 10 | 1.24 |
| (1,2432) | 1:115:A:VAL:HG21 | 1:116:A:GLU:H | 4 | 1.24 |
| (1,2432) | 1:115:A:VAL:HG22 | 1:116:A:GLU:H | 4 | 1.24 |
| (1,2432) | 1:115:A:VAL:HG23 | 1:116:A:GLU:H | 4 | 1.24 |
| (1,1790) | 1:107:A:THR:HG21 | 1:88:A:GLU:HG3 | 4 | 1.24 |
| (1,1790) | 1:107:A:THR:HG22 | 1:88:A:GLU:HG3 | 4 | 1.24 |
| (1,1790) | 1:107:A:THR:HG23 | 1:88:A:GLU:HG3 | 4 | 1.24 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 10 | 1.24 |
| (1,48) | 1:3:A:GLU:HB3 | 1:8:A:THR:HB | 9 | 1.24 |
| (3,31) | 1:75:A:LYS:HE2 | 1:76:A:ARG:H | 8 | 1.23 |
| (1,2773) | 1:10:A:ARG:HG2 | 1:83:A:GLY:H | 1 | 1.23 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 10 | 1.23 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 1 | 1.23 |
| (1,2432) | 1:115:A:VAL:HG21 | 1:116:A:GLU:H | 9 | 1.23 |
| (1,2432) | 1:115:A:VAL:HG22 | 1:116:A:GLU:H | 9 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2432) | 1:115:A:VAL:HG23 | 1:116:A:GLU:H | 9 | 1.23 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 8 | 1.23 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 8 | 1.23 |
| (1,1323) | 1:78:A:LEU:HA | 1:78:A:LEU:HD21 | 6 | 1.23 |
| (1,1323) | 1:78:A:LEU:HA | 1:78:A:LEU:HD22 | 6 | 1.23 |
| (1,1323) | 1:78:A:LEU:HA | 1:78:A:LEU:HD23 | 6 | 1.23 |
| (1,1197) | 1:75:A:LYS:HE3 | 1:71:A:PRO:HB2 | 5 | 1.23 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 10 | 1.23 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 10 | 1.23 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 10 | 1.23 |
| (1,834) | 1:52:A:MET:HG2 | 1:59:A:LEU:HG | 5 | 1.23 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 9 | 1.23 |
| (3,780) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 9 | 1.22 |
| (1,3510) | 1:40:A:LYS:HE2 | 1:41:A:GLU:H | 10 | 1.22 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 4 | 1.22 |
| (1,2324) | 1:126:A:LEU:H | 1:71:A:PRO:HD3 | 10 | 1.22 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 2 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB1 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB2 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB3 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB1 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB2 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB3 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB1 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB2 | 10 | 1.22 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 10 | 1.22 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 1 | 1.22 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 1 | 1.22 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 1 | 1.22 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 5 | 1.22 |
| (1,23) | 1:7:A:ARG:HA | 1:7:A:ARG:HD3 | 2 | 1.22 |
| (3,780) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 4 | 1.21 |
| (3,122) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HG21 | 4 | 1.21 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 3 | 1.21 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 4 | 1.21 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 8 | 1.21 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 2 | 1.21 |
| (1,2432) | 1:115:A:VAL:HG21 | 1:116:A:GLU:H | 8 | 1.21 |
| (1,2432) | 1:115:A:VAL:HG22 | 1:116:A:GLU:H | 8 | 1.21 |
| (1,2432) | 1:115:A:VAL:HG23 | 1:116:A:GLU:H | 8 | 1.21 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 10 | 1.21 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 10 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 10 | 1.21 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 10 | 1.21 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 10 | 1.21 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 10 | 1.21 |
| (1,926) | 1:58:A:LYS:HG3 | 1:59:A:LEU:H | 9 | 1.21 |
| (2,344) | 1:81:A:ASN:HB3 | 1:123:A:ILE:HA | 1 | 1.2 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 10 | 1.2 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 9 | 1.2 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 3 | 1.2 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 10 | 1.2 |
| (1,3541) | 1:81:A:ASN:HD22 | 1:11:A:THR:HB | 5 | 1.2 |
| (1,2720) | 1:88:A:GLU:HG3 | 1:88:A:GLU:H | 1 | 1.2 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 6 | 1.2 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 10 | 1.19 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 3 | 1.19 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 1 | 1.19 |
| (1,2504) | 1:111:A:LYS:HE3 | 1:107:A:THR:H | 9 | 1.19 |
| (1,2420) | 1:115:A:VAL:HG21 | 1:118:A:ILE:H | 8 | 1.19 |
| (1,2420) | 1:115:A:VAL:HG22 | 1:118:A:ILE:H | 8 | 1.19 |
| (1,2420) | 1:115:A:VAL:HG23 | 1:118:A:ILE:H | 8 | 1.19 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 9 | 1.19 |
| (1,1751) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 9 | 1.19 |
| (1,1751) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 9 | 1.19 |
| (1,1751) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 9 | 1.19 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 10 | 1.19 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 10 | 1.19 |
| (1,14) | 1:5:A:LYS:HA | 1:5:A:LYS:HD3 | 6 | 1.19 |
| (3,876) | 1:10:A:ARG:HD2 | 1:81:A:ASN:HD21 | 10 | 1.18 |
| (3,125) | 1:13:A:TYR:HD1 | 1:45:A:LYS:HE3 | 10 | 1.18 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 5 | 1.18 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 9 | 1.18 |
| (1,3758) | 1:65:A:HIS:HE1 | 1:27:A:LYS:HD2 | 8 | 1.18 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 5 | 1.18 |
| (1,2533) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 4 | 1.18 |
| (1,2533) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 4 | 1.18 |
| (1,2533) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 4 | 1.18 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 5 | 1.18 |
| (1,1751) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 8 | 1.18 |
| (1,1751) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 8 | 1.18 |
| (1,1751) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 8 | 1.18 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 5 | 1.18 |
| (1,59) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 2 | 1.18 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1192) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD21 | 6 | 1.17 |
| (3,814) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 2 | 1.17 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 7 | 1.17 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 6 | 1.17 |
| (1,3699) | 1:69:A:VAL:H | 1:70:A:ILE:HG13 | 10 | 1.17 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 8 | 1.17 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 9 | 1.17 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 5 | 1.17 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 5 | 1.17 |
| (1,2432) | 1:115:A:VAL:HG21 | 1:116:A:GLU:H | 6 | 1.17 |
| (1,2432) | 1:115:A:VAL:HG22 | 1:116:A:GLU:H | 6 | 1.17 |
| (1,2432) | 1:115:A:VAL:HG23 | 1:116:A:GLU:H | 6 | 1.17 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 2 | 1.17 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 10 | 1.17 |
| (1,2228) | 1:91:A:LEU:HD21 | 1:103:A:ILE:H | 10 | 1.17 |
| (1,2228) | 1:91:A:LEU:HD22 | 1:103:A:ILE:H | 10 | 1.17 |
| (1,2228) | 1:91:A:LEU:HD23 | 1:103:A:ILE:H | 10 | 1.17 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 8 | 1.17 |
| (1,1926) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 6 | 1.17 |
| (1,1926) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 6 | 1.17 |
| (1,1926) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 6 | 1.17 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 8 | 1.17 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD11 | 1 | 1.16 |
| (3,389) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HG3 | 1 | 1.16 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 1 | 1.16 |
| (1,3755) | 1:34:A:LYS:HE2 | 1:33:A:HIS:HE1 | 7 | 1.16 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 4 | 1.16 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 9 | 1.16 |
| (1,2745) | 1:87:A:ASN:HB3 | 1:86:A:GLY:H | 3 | 1.16 |
| (1,2384) | 1:120:A:TYR:H | 1:121:A:GLU:HB2 | 1 | 1.16 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 8 | 1.16 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 2 | 1.16 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 2 | 1.16 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 2 | 1.16 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 1 | 1.16 |
| (1,2145) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 2 | 1.16 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 9 | 1.16 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 9 | 1.16 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 9 | 1.16 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 5 | 1.16 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 10 | 1.16 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 8 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 9 | 1.16 |
| (3,501) | 1:49:A:VAL:HG13 | 1:40:A:LYS:HB3 | 6 | 1.15 |
| (3,501) | 1:49:A:VAL:HG11 | 1:40:A:LYS:HB3 | 7 | 1.15 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 4 | 1.15 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 2 | 1.15 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 3 | 1.15 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 6 | 1.15 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 2 | 1.15 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 4 | 1.15 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 1 | 1.15 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 1 | 1.15 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 1 | 1.15 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 4 | 1.15 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 4 | 1.15 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 4 | 1.15 |
| (1,1921) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 6 | 1.15 |
| (1,1921) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 6 | 1.15 |
| (1,1921) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 6 | 1.15 |
| (3,501) | 1:49:A:VAL:HG11 | 1:40:A:LYS:HB3 | 5 | 1.14 |
| (2,344) | 1:81:A:ASN:HB3 | 1:123:A:ILE:HA | 4 | 1.14 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 7 | 1.14 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 10 | 1.14 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 7 | 1.14 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 7 | 1.14 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 7 | 1.14 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 8 | 1.14 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 8 | 1.14 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 8 | 1.14 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 5 | 1.14 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 7 | 1.14 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 9 | 1.14 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 2 | 1.13 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 9 | 1.13 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 10 | 1.13 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 3 | 1.13 |
| (1,2995) | 1:60:A:LYS:HE2 | 1:60:A:LYS:H | 10 | 1.13 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 3 | 1.13 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 3 | 1.13 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 8 | 1.13 |
| (1,2591) | 1:95:A:ASN:HB2 | 1:100:A:SER:H | 4 | 1.13 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 10 | 1.13 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 8 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 8 | 1.13 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 8 | 1.13 |
| (1,1921) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 9 | 1.13 |
| (1,1921) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 9 | 1.13 |
| (1,1921) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 9 | 1.13 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 9 | 1.13 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 2 | 1.13 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 10 | 1.13 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 10 | 1.13 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 10 | 1.13 |
| (1,161) | 1:16:A:GLN:HB3 | 1:78:A:LEU:HD11 | 6 | 1.13 |
| (1,161) | 1:16:A:GLN:HB3 | 1:78:A:LEU:HD12 | 6 | 1.13 |
| (1,161) | 1:16:A:GLN:HB3 | 1:78:A:LEU:HD13 | 6 | 1.13 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 2 | 1.12 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 8 | 1.12 |
| (1,2720) | 1:88:A:GLU:HG3 | 1:88:A:GLU:H | 4 | 1.12 |
| (1,2163) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HA | 9 | 1.12 |
| (1,2163) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HA | 9 | 1.12 |
| (1,2163) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HA | 9 | 1.12 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 4 | 1.12 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 4 | 1.12 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 4 | 1.12 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 10 | 1.12 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 10 | 1.12 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 10 | 1.12 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 8 | 1.12 |
| (1,452) | 1:28:A:LEU:HD11 | 1:60:A:LYS:H | 3 | 1.12 |
| (1,452) | 1:28:A:LEU:HD12 | 1:60:A:LYS:H | 3 | 1.12 |
| (1,452) | 1:28:A:LEU:HD13 | 1:60:A:LYS:H | 3 | 1.12 |
| (3,1140) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 9 | 1.11 |
| (3,927) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 1 | 1.11 |
| (3,927) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 10 | 1.11 |
| (3,814) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 1 | 1.11 |
| (3,564) | 1:34:A:LYS:HE2 | 1:34:A:LYS:HG2 | 5 | 1.11 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 4 | 1.11 |
| (3,518) | 1:96:A:GLU:HG3 | 1:97:A:LYS:HG3 | 5 | 1.11 |
| (3,299) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 10 | 1.11 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 3 | 1.11 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 8 | 1.11 |
| (1,3641) | 1:11:A:THR:H | 1:81:A:ASN:HD21 | 5 | 1.11 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 3 | 1.11 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 1 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 5 | 1.11 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 7 | 1.11 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 5 | 1.11 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 3 | 1.11 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 9 | 1.11 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 8 | 1.11 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 6 | 1.11 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 6 | 1.11 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 6 | 1.11 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 10 | 1.11 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 10 | 1.11 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 10 | 1.11 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 2 | 1.11 |
| (1,2144) | 1:119:A:GLN:HB3 | 1:122:A:ASP:HB3 | 2 | 1.11 |
| (1,1751) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 10 | 1.11 |
| (1,1751) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 10 | 1.11 |
| (1,1751) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 10 | 1.11 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 4 | 1.11 |
| (3,927) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 2 | 1.1 |
| (3,927) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 3 | 1.1 |
| (3,927) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 4 | 1.1 |
| (3,927) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 6 | 1.1 |
| (3,927) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 7 | 1.1 |
| (3,927) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 8 | 1.1 |
| (3,564) | 1:34:A:LYS:HE2 | 1:34:A:LYS:HG2 | 4 | 1.1 |
| (3,564) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 9 | 1.1 |
| (3,401) | 1:15:A:LEU:HD23 | 1:66:A:LEU:HD23 | 9 | 1.1 |
| (3,317) | 1:34:A:LYS:HE3 | 1:34:A:LYS:HB3 | 7 | 1.1 |
| (3,31) | 1:75:A:LYS:HE2 | 1:76:A:ARG:H | 2 | 1.1 |
| (2,590) | 1:7:A:ARG:HB2 | 1:9:A:ALA:H | 8 | 1.1 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 5 | 1.1 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 8 | 1.1 |
| (1,3630) | 1:123:A:ILE:H | 1:80:A:LEU:HB3 | 1 | 1.1 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 3 | 1.1 |
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 3 | 1.1 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 4 | 1.1 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 4 | 1.1 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 4 | 1.1 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 9 | 1.1 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 9 | 1.1 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 9 | 1.1 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 9 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 9 | 1.1 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 9 | 1.1 |
| (3,927) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 5 | 1.09 |
| (3,927) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 9 | 1.09 |
| (3,814) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 8 | 1.09 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 10 | 1.09 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 2 | 1.09 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG21 | 3 | 1.09 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG22 | 3 | 1.09 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG23 | 3 | 1.09 |
| (1,2163) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HA | 10 | 1.09 |
| (1,2163) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HA | 10 | 1.09 |
| (1,2163) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HA | 10 | 1.09 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 9 | 1.09 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 9 | 1.09 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 9 | 1.09 |
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 5 | 1.09 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 5 | 1.09 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 5 | 1.09 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 2 | 1.09 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 7 | 1.08 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 4 | 1.08 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 1 | 1.08 |
| (1,2420) | 1:115:A:VAL:HG21 | 1:118:A:ILE:H | 6 | 1.08 |
| (1,2420) | 1:115:A:VAL:HG22 | 1:118:A:ILE:H | 6 | 1.08 |
| (1,2420) | 1:115:A:VAL:HG23 | 1:118:A:ILE:H | 6 | 1.08 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 7 | 1.08 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 10 | 1.08 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 10 | 1.08 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 10 | 1.08 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 3 | 1.08 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 2 | 1.08 |
| (1,1317) | 1:31:A:LYS:HG2 | 1:32:A:TYR:H | 1 | 1.08 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 3 | 1.08 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 10 | 1.08 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 1 | 1.08 |
| (1,75) | 1:11:A:THR:HB | 1:13:A:TYR:HD1 | 4 | 1.08 |
| (1,75) | 1:11:A:THR:HB | 1:13:A:TYR:HD2 | 4 | 1.08 |
| (3,564) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 6 | 1.07 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 2 | 1.07 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 6 | 1.07 |
| (1,3557) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HD21 | 10 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 6 | 1.07 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 9 | 1.07 |
| (1,2163) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HA | 6 | 1.07 |
| (1,2163) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HA | 6 | 1.07 |
| (1,2163) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HA | 6 | 1.07 |
| (1,1927) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 9 | 1.07 |
| (1,1927) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 9 | 1.07 |
| (1,1927) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 9 | 1.07 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 3 | 1.07 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 3 | 1.07 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 3 | 1.07 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 10 | 1.07 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 10 | 1.07 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 10 | 1.07 |
| (3,1140) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 4 | 1.06 |
| (3,563) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 4 | 1.06 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 5 | 1.06 |
| (1,3509) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 10 | 1.06 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 7 | 1.06 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 3 | 1.06 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 3 | 1.06 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 6 | 1.06 |
| (1,1927) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 8 | 1.06 |
| (1,1927) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 8 | 1.06 |
| (1,1927) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 8 | 1.06 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 6 | 1.06 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 9 | 1.06 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 9 | 1.06 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 9 | 1.06 |
| (3,564) | 1:34:A:LYS:HE2 | 1:34:A:LYS:HG2 | 7 | 1.05 |
| (3,563) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 1 | 1.05 |
| (3,563) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 9 | 1.05 |
| (3,563) | 1:58:A:LYS:HG2 | 1:58:A:LYS:HE2 | 10 | 1.05 |
| (2,611) | 1:123:A:ILE:H | 1:81:A:ASN:HB3 | 9 | 1.05 |
| (1,3253) | 1:31:A:LYS:HG2 | 1:32:A:TYR:H | 1 | 1.05 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 2 | 1.05 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 6 | 1.05 |
| (1,2533) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 6 | 1.05 |
| (1,2533) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 6 | 1.05 |
| (1,2533) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 6 | 1.05 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 5 | 1.05 |
| (1,1898) | 1:115:A:VAL:H | 1:114:A:ARG:HG2 | 10 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1751) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 4 | 1.05 |
| (1,1751) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 4 | 1.05 |
| (1,1751) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 4 | 1.05 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 6 | 1.05 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 7 | 1.05 |
| (1,48) | 1:3:A:GLU:HB3 | 1:8:A:THR:HB | 10 | 1.05 |
| (3,563) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 2 | 1.04 |
| (3,563) | 1:58:A:LYS:HG2 | 1:58:A:LYS:HE2 | 7 | 1.04 |
| (3,389) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HG3 | 6 | 1.04 |
| (3,31) | 1:75:A:LYS:HE3 | 1:76:A:ARG:H | 10 | 1.04 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 10 | 1.04 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 7 | 1.04 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 5 | 1.04 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 6 | 1.04 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 10 | 1.04 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 10 | 1.04 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 10 | 1.04 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 7 | 1.04 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 3 | 1.04 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 3 | 1.04 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 3 | 1.04 |
| (1,1921) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 4 | 1.04 |
| (1,1921) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 4 | 1.04 |
| (1,1921) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 4 | 1.04 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 8 | 1.04 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 8 | 1.04 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 8 | 1.04 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 4 | 1.04 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 4 | 1.04 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 4 | 1.04 |
| (1,956) | 1:60:A:LYS:HB3 | 1:49:A:VAL:HA | 1 | 1.04 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 10 | 1.04 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 10 | 1.04 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 10 | 1.04 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 5 | 1.03 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 1 | 1.03 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 10 | 1.03 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 1 | 1.03 |
| (1,2163) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HA | 8 | 1.03 |
| (1,2163) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HA | 8 | 1.03 |
| (1,2163) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HA | 8 | 1.03 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 6 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,22) | 1:125:A:LYS:HG2 | 1:20:A:ILE:HD11 | 8 | 1.03 |
| (1,22) | 1:125:A:LYS:HG2 | 1:20:A:ILE:HD12 | 8 | 1.03 |
| (1,22) | 1:125:A:LYS:HG2 | 1:20:A:ILE:HD13 | 8 | 1.03 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 3 | 1.02 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 1 | 1.02 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 8 | 1.02 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 10 | 1.02 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 7 | 1.02 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 8 | 1.02 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 5 | 1.02 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 8 | 1.02 |
| (1,1317) | 1:31:A:LYS:HG2 | 1:32:A:TYR:H | 5 | 1.02 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 6 | 1.02 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 6 | 1.02 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 6 | 1.02 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 6 | 1.02 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 6 | 1.02 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 6 | 1.02 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 2 | 1.02 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 3 | 1.02 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 7 | 1.02 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 3 | 1.02 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 3 | 1.02 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 3 | 1.02 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 3 | 1.02 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 3 | 1.02 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 3 | 1.02 |
| (3,635) | 1:23:A:ILE:HG22 | 1:24:A:ILE:H | 6 | 1.01 |
| (2,344) | 1:81:A:ASN:HB3 | 1:123:A:ILE:HA | 3 | 1.01 |
| (1,3837) | 1:11:A:THR:HB | 1:13:A:TYR:HE1 | 4 | 1.01 |
| (1,3837) | 1:11:A:THR:HB | 1:13:A:TYR:HE2 | 4 | 1.01 |
| (1,2604) | 1:95:A:ASN:HB2 | 1:99:A:PHE:H | 4 | 1.01 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG11 | 8 | 1.01 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG12 | 8 | 1.01 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG13 | 8 | 1.01 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 9 | 1.01 |
| (1,1886) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 10 | 1.01 |
| (1,1886) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 10 | 1.01 |
| (1,1886) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 10 | 1.01 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 5 | 1.01 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 5 | 1.01 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 5 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 5 | 1.01 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 6 | 1.01 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 6 | 1.01 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 6 | 1.01 |
| (1,1419) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HB3 | 9 | 1.01 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 5 | 1.01 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 8 | 1.01 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 9 | 1.01 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD12 | 5 | 1.0 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 1 | 1.0 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 8 | 1.0 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 8 | 1.0 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 8 | 1.0 |
| (1,3837) | 1:11:A:THR:HB | 1:13:A:TYR:HE1 | 3 | 1.0 |
| (1,3837) | 1:11:A:THR:HB | 1:13:A:TYR:HE2 | 3 | 1.0 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 9 | 1.0 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 9 | 1.0 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 3 | 1.0 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 3 | 1.0 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 9 | 1.0 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 7 | 1.0 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG21 | 3 | 1.0 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG22 | 3 | 1.0 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG23 | 3 | 1.0 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 7 | 1.0 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 8 | 1.0 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 10 | 1.0 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 5 | 1.0 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 6 | 1.0 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 7 | 1.0 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 7 | 1.0 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 7 | 1.0 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 4 | 1.0 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 1 | 1.0 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 1 | 1.0 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 1 | 1.0 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG21 | 4 | 0.99 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG22 | 4 | 0.99 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG23 | 4 | 0.99 |
| (1,3253) | 1:31:A:LYS:HG2 | 1:32:A:TYR:H | 5 | 0.99 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 1 | 0.99 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 4 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 9 | 0.99 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 4 | 0.99 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 4 | 0.99 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 4 | 0.99 |
| (1,1927) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 10 | 0.99 |
| (1,1927) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 10 | 0.99 |
| (1,1927) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 10 | 0.99 |
| (1,1729) | 1:106:A:GLU:HG2 | 1:105:A:ILE:HA | 3 | 0.99 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 6 | 0.99 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 10 | 0.99 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 5 | 0.99 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 5 | 0.99 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 5 | 0.99 |
| (3,814) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 5 | 0.98 |
| (3,583) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB3 | 1 | 0.98 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD11 | 3 | 0.98 |
| (3,564) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 1 | 0.98 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 2 | 0.98 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 6 | 0.98 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 9 | 0.98 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 2 | 0.98 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 1 | 0.98 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 3 | 0.98 |
| (1,2620) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 4 | 0.98 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 6 | 0.98 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 6 | 0.98 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 6 | 0.98 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 7 | 0.98 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 8 | 0.98 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 8 | 0.98 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 8 | 0.98 |
| (1,958) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 1 | 0.98 |
| (1,14) | 1:5:A:LYS:HA | 1:5:A:LYS:HD2 | 3 | 0.98 |
| (3,1144) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 9 | 0.97 |
| (3,857) | 1:114:A:ARG:HB3 | 1:115:A:VAL:HG13 | 9 | 0.97 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 5 | 0.97 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD12 | 7 | 0.97 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 5 | 0.97 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 8 | 0.97 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 8 | 0.97 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 7 | 0.97 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 7 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 7 | 0.97 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 6 | 0.97 |
| (1,2092) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HG13 | 2 | 0.97 |
| (1,2092) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HG13 | 2 | 0.97 |
| (1,2092) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HG13 | 2 | 0.97 |
| (1,1915) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 10 | 0.97 |
| (1,1915) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 10 | 0.97 |
| (1,1915) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 10 | 0.97 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 4 | 0.97 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD11 | 10 | 0.97 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD12 | 10 | 0.97 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD13 | 10 | 0.97 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 3 | 0.96 |
| (3,401) | 1:15:A:LEU:HD22 | 1:80:A:LEU:HD13 | 3 | 0.96 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 7 | 0.96 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 7 | 0.96 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 7 | 0.96 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 6 | 0.96 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 5 | 0.96 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 5 | 0.96 |
| (1,3331) | 1:20:A:ILE:H | 1:124:A:SER:HB3 | 1 | 0.96 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 5 | 0.96 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 5 | 0.96 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 5 | 0.96 |
| (1,1915) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 4 | 0.96 |
| (1,1915) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 4 | 0.96 |
| (1,1915) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 4 | 0.96 |
| (1,1886) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 8 | 0.96 |
| (1,1886) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 8 | 0.96 |
| (1,1886) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 8 | 0.96 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 6 | 0.96 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 3 | 0.96 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 3 | 0.96 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 3 | 0.96 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 3 | 0.96 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 3 | 0.96 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 3 | 0.96 |
| (1,596) | 1:49:A:VAL:HB | 1:40:A:LYS:HB3 | 1 | 0.96 |
| (3,1156) | 1:9:A:ALA:HB2 | 1:10:A:ARG:H | 3 | 0.95 |
| (3,177) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HA | 9 | 0.95 |
| (2,602) | 1:60:A:LYS:HE2 | 1:59:A:LEU:H | 4 | 0.95 |
| (2,249) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB2 | 4 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 10 | 0.95 |
| (1,2737) | 1:78:A:LEU:HD21 | 1:87:A:ASN:H | 6 | 0.95 |
| (1,2737) | 1:78:A:LEU:HD22 | 1:87:A:ASN:H | 6 | 0.95 |
| (1,2737) | 1:78:A:LEU:HD23 | 1:87:A:ASN:H | 6 | 0.95 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 4 | 0.95 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 9 | 0.95 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 9 | 0.95 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 9 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 6 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 6 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 6 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 8 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 8 | 0.95 |
| (1,1915) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 8 | 0.95 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 9 | 0.95 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 9 | 0.95 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 6 | 0.95 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 6 | 0.95 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 6 | 0.95 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 7 | 0.95 |
| (3,857) | 1:114:A:ARG:HB3 | 1:115:A:VAL:HG13 | 8 | 0.94 |
| (3,814) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 3 | 0.94 |
| (3,603) | 1:25:A:THR:HG21 | 1:23:A:ILE:HD12 | 3 | 0.94 |
| (3,501) | 1:49:A:VAL:HG11 | 1:40:A:LYS:HB3 | 2 | 0.94 |
| (3,501) | 1:49:A:VAL:HG12 | 1:40:A:LYS:HB3 | 8 | 0.94 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 9 | 0.94 |
| (2,479) | 1:102:A:THR:H | 1:100:A:SER:HB3 | 3 | 0.94 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 7 | 0.94 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 8 | 0.94 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 7 | 0.94 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 6 | 0.94 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 9 | 0.94 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 3 | 0.94 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 2 | 0.94 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 4 | 0.94 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 4 | 0.94 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 4 | 0.94 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 6 | 0.94 |
| (1,281) | 1:20:A:ILE:HD11 | 1:20:A:ILE:HB | 8 | 0.94 |
| (1,281) | 1:20:A:ILE:HD12 | 1:20:A:ILE:HB | 8 | 0.94 |
| (1,281) | 1:20:A:ILE:HD13 | 1:20:A:ILE:HB | 8 | 0.94 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 6 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 1 | 0.93 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 10 | 0.93 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 2 | 0.93 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 10 | 0.93 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 10 | 0.93 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 10 | 0.93 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 1 | 0.93 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG11 | 6 | 0.93 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG12 | 6 | 0.93 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG13 | 6 | 0.93 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 9 | 0.93 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 3 | 0.93 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 3 | 0.93 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 3 | 0.93 |
| (1,2163) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HA | 4 | 0.93 |
| (1,2163) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HA | 4 | 0.93 |
| (1,2163) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HA | 4 | 0.93 |
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 10 | 0.93 |
| (1,1915) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 9 | 0.93 |
| (1,1915) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 9 | 0.93 |
| (1,1915) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 9 | 0.93 |
| (1,1906) | 1:115:A:VAL:HA | 1:116:A:GLU:HG2 | 1 | 0.93 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 7 | 0.93 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 9 | 0.93 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 9 | 0.93 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 9 | 0.93 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HG2 | 8 | 0.92 |
| (3,1144) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 4 | 0.92 |
| (3,814) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 9 | 0.92 |
| (3,466) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 8 | 0.92 |
| (3,177) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HA | 1 | 0.92 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 6 | 0.92 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 6 | 0.92 |
| (1,3648) | 1:16:A:GLN:HE22 | 1:80:A:LEU:HG | 10 | 0.92 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 6 | 0.92 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 6 | 0.92 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 9 | 0.92 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 4 | 0.92 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 9 | 0.92 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 9 | 0.92 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 9 | 0.92 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 6 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 2 | 0.92 |
| (1,1927) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 4 | 0.92 |
| (1,1927) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 4 | 0.92 |
| (1,1927) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 4 | 0.92 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 1 | 0.92 |
| (1,1751) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 6 | 0.92 |
| (1,1751) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 6 | 0.92 |
| (1,1751) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 6 | 0.92 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 6 | 0.92 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 10 | 0.92 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 10 | 0.92 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 10 | 0.92 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 2 | 0.92 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG22 | 2 | 0.91 |
| (3,186) | 1:52:A:MET:HG3 | 1:59:A:LEU:H | 4 | 0.91 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 4 | 0.91 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 4 | 0.91 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 4 | 0.91 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 2 | 0.91 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 5 | 0.91 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 5 | 0.91 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 2 | 0.91 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 2 | 0.91 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 2 | 0.91 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 8 | 0.91 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 2 | 0.91 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 3 | 0.91 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 7 | 0.91 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 9 | 0.91 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 1 | 0.91 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 1 | 0.91 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 1 | 0.91 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 2 | 0.91 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 2 | 0.91 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 2 | 0.91 |
| (3,876) | 1:10:A:ARG:HD2 | 1:81:A:ASN:HD21 | 2 | 0.9 |
| (3,603) | 1:25:A:THR:HG21 | 1:23:A:ILE:HD13 | 7 | 0.9 |
| (3,389) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HG3 | 3 | 0.9 |
| (2,611) | 1:123:A:ILE:H | 1:81:A:ASN:HB3 | 1 | 0.9 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 4 | 0.9 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 4 | 0.9 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 4 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2153) | 1:118:A:ILE:HA | 1:100:A:SER:HB2 | 9 | 0.9 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 6 | 0.9 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 6 | 0.9 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 6 | 0.9 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 2 | 0.9 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 2 | 0.9 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 2 | 0.9 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 6 | 0.9 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 6 | 0.9 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 6 | 0.9 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 4 | 0.9 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 5 | 0.9 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 8 | 0.9 |
| (3,892) | 1:25:A:THR:HG21 | 1:25:A:THR:HA | 1 | 0.89 |
| (3,814) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 4 | 0.89 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 9 | 0.89 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 9 | 0.89 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 9 | 0.89 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 5 | 0.89 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 2 | 0.89 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 6 | 0.89 |
| (1,3560) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 2 | 0.89 |
| (1,3382) | 1:14:A:TRP:H | 1:15:A:LEU:HB3 | 8 | 0.89 |
| (1,3121) | 1:45:A:LYS:H | 1:45:A:LYS:HG3 | 2 | 0.89 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 5 | 0.89 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 3 | 0.89 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 4 | 0.89 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 1 | 0.89 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 6 | 0.89 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 10 | 0.89 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 5 | 0.89 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 5 | 0.89 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 5 | 0.89 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 3 | 0.89 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 3 | 0.89 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 3 | 0.89 |
| (3,892) | 1:25:A:THR:HG21 | 1:25:A:THR:HA | 2 | 0.88 |
| (3,892) | 1:25:A:THR:HG22 | 1:25:A:THR:HA | 8 | 0.88 |
| (3,892) | 1:25:A:THR:HG23 | 1:25:A:THR:HA | 9 | 0.88 |
| (3,401) | 1:15:A:LEU:HD21 | 1:80:A:LEU:HD12 | 6 | 0.88 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD12 | 8 | 0.88 |
| (3,31) | 1:75:A:LYS:HE3 | 1:76:A:ARG:H | 5 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 2 | 0.88 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 2 | 0.88 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 2 | 0.88 |
| (1,2861) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 10 | 0.88 |
| (1,2861) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 10 | 0.88 |
| (1,2861) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 10 | 0.88 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 1 | 0.88 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 5 | 0.88 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 8 | 0.88 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 8 | 0.88 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 8 | 0.88 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 9 | 0.88 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 9 | 0.88 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 9 | 0.88 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 8 | 0.88 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 1 | 0.88 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 1 | 0.88 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 1 | 0.88 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 8 | 0.88 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 8 | 0.88 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 8 | 0.88 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 6 | 0.88 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 6 | 0.88 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 6 | 0.88 |
| (3,892) | 1:25:A:THR:HG22 | 1:25:A:THR:HA | 4 | 0.87 |
| (3,892) | 1:25:A:THR:HG22 | 1:25:A:THR:HA | 5 | 0.87 |
| (3,876) | 1:10:A:ARG:HD3 | 1:81:A:ASN:HD21 | 7 | 0.87 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 6 | 0.87 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG23 | 9 | 0.87 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD11 | 8 | 0.87 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 7 | 0.87 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 7 | 0.87 |
| (1,3493) | 1:26:A:LYS:HB2 | 1:33:A:HIS:H | 6 | 0.87 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE3 | 4 | 0.87 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 8 | 0.87 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 5 | 0.87 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 8 | 0.87 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 4 | 0.87 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 7 | 0.87 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 6 | 0.87 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 5 | 0.87 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 5 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 5 | 0.87 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 4 | 0.87 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 1 | 0.87 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 2 | 0.87 |
| (1,915) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HB3 | 1 | 0.87 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 3 | 0.87 |
| (3,892) | 1:25:A:THR:HG23 | 1:25:A:THR:HA | 3 | 0.86 |
| (3,892) | 1:25:A:THR:HG23 | 1:25:A:THR:HA | 7 | 0.86 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG23 | 6 | 0.86 |
| (3,339) | 1:30:A:GLU:HG2 | 1:32:A:TYR:H | 6 | 0.86 |
| (3,241) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HE22 | 1 | 0.86 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 4 | 0.86 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 7 | 0.86 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 9 | 0.86 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 9 | 0.86 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 3 | 0.86 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 9 | 0.86 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 3 | 0.86 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 4 | 0.86 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 8 | 0.86 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 10 | 0.86 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 4 | 0.86 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 9 | 0.86 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 6 | 0.86 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 4 | 0.86 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 9 | 0.86 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 5 | 0.86 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 10 | 0.86 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 10 | 0.86 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 4 | 0.86 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 4 | 0.86 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 4 | 0.86 |
| (1,1733) | 1:122:A:ASP:H | 1:121:A:GLU:HG3 | 3 | 0.86 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 7 | 0.86 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 2 | 0.86 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 10 | 0.86 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 6 | 0.86 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 6 | 0.86 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 6 | 0.86 |
| (1,59) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 10 | 0.86 |
| (3,615) | 1:105:A:ILE:HA | 1:87:A:ASN:HB2 | 2 | 0.85 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD11 | 2 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB3 | 10 | 0.85 |
| (2,366) | 1:107:A:THR:HB | 1:88:A:GLU:HG3 | 1 | 0.85 |
| (2,365) | 1:107:A:THR:HB | 1:88:A:GLU:HG3 | 1 | 0.85 |
| (1,3579) | 1:84:A:TYR:HB2 | 1:87:A:ASN:HD22 | 9 | 0.85 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 6 | 0.85 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 9 | 0.85 |
| (1,2621) | 1:97:A:LYS:H | 1:97:A:LYS:HD3 | 10 | 0.85 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 4 | 0.85 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 7 | 0.85 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 9 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG11 | 4 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG12 | 4 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG13 | 4 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG11 | 9 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG12 | 9 | 0.85 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG13 | 9 | 0.85 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 4 | 0.85 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 6 | 0.85 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 5 | 0.85 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 8 | 0.85 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 10 | 0.85 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 6 | 0.85 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 2 | 0.85 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 2 | 0.85 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 2 | 0.85 |
| (1,1886) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 6 | 0.85 |
| (1,1886) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 6 | 0.85 |
| (1,1886) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 6 | 0.85 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 9 | 0.85 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 9 | 0.85 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 9 | 0.85 |
| (1,1840) | 1:110:A:LEU:H | 1:110:A:LEU:HD11 | 10 | 0.85 |
| (1,1840) | 1:110:A:LEU:H | 1:110:A:LEU:HD12 | 10 | 0.85 |
| (1,1840) | 1:110:A:LEU:H | 1:110:A:LEU:HD13 | 10 | 0.85 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 4 | 0.85 |
| (1,1465) | 1:78:A:LEU:HD21 | 1:88:A:GLU:HA | 6 | 0.85 |
| (1,1465) | 1:78:A:LEU:HD22 | 1:88:A:GLU:HA | 6 | 0.85 |
| (1,1465) | 1:78:A:LEU:HD23 | 1:88:A:GLU:HA | 6 | 0.85 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 8 | 0.85 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 8 | 0.85 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 8 | 0.85 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 5 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,581) | 1:78:A:LEU:HD21 | 1:88:A:GLU:HA | 6 | 0.85 |
| (1,581) | 1:78:A:LEU:HD22 | 1:88:A:GLU:HA | 6 | 0.85 |
| (1,581) | 1:78:A:LEU:HD23 | 1:88:A:GLU:HA | 6 | 0.85 |
| (1,75) | 1:11:A:THR:HB | 1:13:A:TYR:HD1 | 3 | 0.85 |
| (1,75) | 1:11:A:THR:HB | 1:13:A:TYR:HD2 | 3 | 0.85 |
| (3,850) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HH2 | 3 | 0.84 |
| (3,850) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HH2 | 5 | 0.84 |
| (3,850) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HH2 | 10 | 0.84 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG22 | 5 | 0.84 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG22 | 3 | 0.84 |
| (3,125) | 1:44:A:ASP:HB2 | 1:46:A:TYR:HD2 | 1 | 0.84 |
| (1,3758) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 1 | 0.84 |
| (1,3726) | 1:95:A:ASN:HD21 | 1:98:A:THR:HB | 8 | 0.84 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 8 | 0.84 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 2 | 0.84 |
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 4 | 0.84 |
| (1,2584) | 1:100:A:SER:H | 1:119:A:GLN:HE22 | 6 | 0.84 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 8 | 0.84 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 10 | 0.84 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 1 | 0.84 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 2 | 0.84 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 3 | 0.84 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 8 | 0.84 |
| (1,1958) | 1:118:A:ILE:HD11 | 1:118:A:ILE:HA | 6 | 0.84 |
| (1,1958) | 1:118:A:ILE:HD12 | 1:118:A:ILE:HA | 6 | 0.84 |
| (1,1958) | 1:118:A:ILE:HD13 | 1:118:A:ILE:HA | 6 | 0.84 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 2 | 0.84 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 2 | 0.84 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 2 | 0.84 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 10 | 0.84 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 2 | 0.84 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 2 | 0.84 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 2 | 0.84 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 8 | 0.84 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 7 | 0.84 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 7 | 0.84 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 7 | 0.84 |
| (3,995) | 1:79:A:VAL:HG22 | 1:79:A:VAL:H | 1 | 0.83 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD12 | 10 | 0.83 |
| (3,635) | 1:23:A:ILE:HG22 | 1:24:A:ILE:H | 10 | 0.83 |
| (3,603) | 1:25:A:THR:HG23 | 1:23:A:ILE:HD11 | 8 | 0.83 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 1 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,399) | 1:43:A:ILE:HG22 | 1:44:A:ASP:HA | 2 | 0.83 |
| (2,611) | 1:123:A:ILE:H | 1:81:A:ASN:HB3 | 4 | 0.83 |
| (2,366) | 1:107:A:THR:HB | 1:88:A:GLU:HG3 | 4 | 0.83 |
| (2,365) | 1:107:A:THR:HB | 1:88:A:GLU:HG3 | 4 | 0.83 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 8 | 0.83 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 8 | 0.83 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 2 | 0.83 |
| (1,2784) | 1:82:A:GLY:H | 1:10:A:ARG:HG2 | 2 | 0.83 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 3 | 0.83 |
| (1,2491) | 1:110:A:LEU:HB3 | 1:110:A:LEU:H | 2 | 0.83 |
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 2 | 0.83 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 8 | 0.83 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 10 | 0.83 |
| (1,1886) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 9 | 0.83 |
| (1,1886) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 9 | 0.83 |
| (1,1886) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 9 | 0.83 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 3 | 0.83 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 7 | 0.83 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 7 | 0.83 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 7 | 0.83 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 8 | 0.83 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 8 | 0.83 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 8 | 0.83 |
| (3,995) | 1:102:A:THR:HG23 | 1:116:A:GLU:H | 6 | 0.82 |
| (3,892) | 1:25:A:THR:HG21 | 1:25:A:THR:HA | 6 | 0.82 |
| (3,857) | 1:115:A:VAL:HG13 | 1:114:A:ARG:HB2 | 6 | 0.82 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 2 | 0.82 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 10 | 0.82 |
| (3,501) | 1:49:A:VAL:HG13 | 1:40:A:LYS:HB3 | 3 | 0.82 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG21 | 7 | 0.82 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 10 | 0.82 |
| (2,349) | 1:118:A:ILE:HG12 | 1:84:A:TYR:HB3 | 8 | 0.82 |
| (2,182) | 1:91:A:LEU:HD11 | 1:72:A:ALA:H | 10 | 0.82 |
| (2,182) | 1:91:A:LEU:HD12 | 1:72:A:ALA:H | 10 | 0.82 |
| (2,182) | 1:91:A:LEU:HD13 | 1:72:A:ALA:H | 10 | 0.82 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 10 | 0.82 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 10 | 0.82 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 6 | 0.82 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 7 | 0.82 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 1 | 0.82 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 5 | 0.82 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 6 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2366) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 6 | 0.82 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 7 | 0.82 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 2 | 0.82 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 4 | 0.82 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 7 | 0.82 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 7 | 0.82 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 7 | 0.82 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 10 | 0.82 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 8 | 0.82 |
| (1,547) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HB | 9 | 0.82 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 3 | 0.82 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 3 | 0.82 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 3 | 0.82 |
| (3,995) | 1:102:A:THR:HG22 | 1:116:A:GLU:H | 8 | 0.81 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD12 | 10 | 0.81 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD12 | 4 | 0.81 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB2 | 5 | 0.81 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 8 | 0.81 |
| (1,3652) | 1:22:A:LYS:H | 1:22:A:LYS:HE2 | 2 | 0.81 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 1 | 0.81 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 1 | 0.81 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 5 | 0.81 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 7 | 0.81 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 8 | 0.81 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HG22 | 4 | 0.8 |
| (3,1087) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HB3 | 7 | 0.8 |
| (3,1087) | 1:61:A:LEU:HD12 | 1:59:A:LEU:HB3 | 7 | 0.8 |
| (3,1087) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HB3 | 7 | 0.8 |
| (3,892) | 1:25:A:THR:HG22 | 1:25:A:THR:HA | 10 | 0.8 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD11 | 2 | 0.8 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 3 | 0.8 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 9 | 0.8 |
| (1,3599) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD22 | 9 | 0.8 |
| (1,3599) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD22 | 9 | 0.8 |
| (1,3599) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD22 | 9 | 0.8 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 9 | 0.8 |
| (1,3580) | 1:110:A:LEU:HD21 | 1:87:A:ASN:HD22 | 10 | 0.8 |
| (1,3580) | 1:110:A:LEU:HD22 | 1:87:A:ASN:HD22 | 10 | 0.8 |
| (1,3580) | 1:110:A:LEU:HD23 | 1:87:A:ASN:HD22 | 10 | 0.8 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 1 | 0.8 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 1 | 0.8 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 1 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2865) | 1:75:A:LYS:H | 1:71:A:PRO:HB2 | 10 | 0.8 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 2 | 0.8 |
| (1,2201) | 1:105:A:ILE:HG21 | 1:84:A:TYR:HB2 | 3 | 0.8 |
| (1,2201) | 1:105:A:ILE:HG22 | 1:84:A:TYR:HB2 | 3 | 0.8 |
| (1,2201) | 1:105:A:ILE:HG23 | 1:84:A:TYR:HB2 | 3 | 0.8 |
| (1,2096) | 1:125:A:LYS:HE2 | 1:127:A:ALA:HA | 2 | 0.8 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 9 | 0.8 |
| (1,1927) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG12 | 6 | 0.8 |
| (1,1927) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG12 | 6 | 0.8 |
| (1,1927) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG12 | 6 | 0.8 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 1 | 0.8 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 1 | 0.8 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 1 | 0.8 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 1 | 0.8 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 1 | 0.8 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 1 | 0.8 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 1 | 0.8 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 1 | 0.8 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 6 | 0.8 |
| (1,1617) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 4 | 0.8 |
| (1,1617) | 1:98:A:THR:HG22 | 1:98:A:THR:HA | 4 | 0.8 |
| (1,1617) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 4 | 0.8 |
| (1,1617) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 6 | 0.8 |
| (1,1617) | 1:98:A:THR:HG22 | 1:98:A:THR:HA | 6 | 0.8 |
| (1,1617) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 6 | 0.8 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 7 | 0.8 |
| (1,1224) | 1:73:A:PRO:HA | 1:91:A:LEU:HD11 | 10 | 0.8 |
| (1,1224) | 1:73:A:PRO:HA | 1:91:A:LEU:HD12 | 10 | 0.8 |
| (1,1224) | 1:73:A:PRO:HA | 1:91:A:LEU:HD13 | 10 | 0.8 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 2 | 0.8 |
| (3,603) | 1:25:A:THR:HG23 | 1:23:A:ILE:HD13 | 9 | 0.79 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD12 | 5 | 0.79 |
| (3,379) | 1:45:A:LYS:HA | 1:46:A:TYR:HD2 | 9 | 0.79 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 10 | 0.79 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 5 | 0.79 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 8 | 0.79 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 4 | 0.79 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 9 | 0.79 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 9 | 0.79 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 9 | 0.79 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 5 | 0.79 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 5 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 5 | 0.79 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 1 | 0.79 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 4 | 0.79 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 9 | 0.79 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 3 | 0.79 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 6 | 0.79 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 1 | 0.79 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 3 | 0.79 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 3 | 0.79 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 9 | 0.79 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 9 | 0.79 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 9 | 0.79 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 1 | 0.79 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 1 | 0.79 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 1 | 0.79 |
| (1,561) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 9 | 0.79 |
| (1,561) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 9 | 0.79 |
| (1,561) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 9 | 0.79 |
| (1,467) | 1:30:A:GLU:HG2 | 1:30:A:GLU:HA | 5 | 0.79 |
| (1,467) | 1:30:A:GLU:HG2 | 1:30:A:GLU:HA | 7 | 0.79 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 10 | 0.78 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG21 | 4 | 0.78 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG21 | 10 | 0.78 |
| (3,603) | 1:25:A:THR:HG23 | 1:23:A:ILE:HD13 | 4 | 0.78 |
| (3,399) | 1:43:A:ILE:HG22 | 1:44:A:ASP:HA | 8 | 0.78 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 1 | 0.78 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 1 | 0.78 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 1 | 0.78 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 5 | 0.78 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 6 | 0.78 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 8 | 0.78 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 3 | 0.78 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 5 | 0.78 |
| (1,2554) | 1:91:A:LEU:HD21 | 1:102:A:THR:H | 10 | 0.78 |
| (1,2554) | 1:91:A:LEU:HD22 | 1:102:A:THR:H | 10 | 0.78 |
| (1,2554) | 1:91:A:LEU:HD23 | 1:102:A:THR:H | 10 | 0.78 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 6 | 0.78 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 10 | 0.78 |
| (1,1933) | 1:115:A:VAL:HG21 | 1:116:A:GLU:HA | 10 | 0.78 |
| (1,1933) | 1:115:A:VAL:HG22 | 1:116:A:GLU:HA | 10 | 0.78 |
| (1,1933) | 1:115:A:VAL:HG23 | 1:116:A:GLU:HA | 10 | 0.78 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 3 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 3 | 0.78 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 3 | 0.78 |
| (1,1197) | 1:75:A:LYS:HE3 | 1:71:A:PRO:HB2 | 2 | 0.78 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 6 | 0.78 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 6 | 0.78 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 8 | 0.78 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 8 | 0.78 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 8 | 0.78 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 7 | 0.78 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 7 | 0.78 |
| (1,467) | 1:30:A:GLU:HG2 | 1:30:A:GLU:HA | 8 | 0.78 |
| (3,1164) | 1:28:A:LEU:HD22 | 1:29:A:GLY:H | 2 | 0.77 |
| (3,1164) | 1:28:A:LEU:HD22 | 1:29:A:GLY:H | 10 | 0.77 |
| (3,857) | 1:115:A:VAL:HG13 | 1:114:A:ARG:HB2 | 4 | 0.77 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG22 | 7 | 0.77 |
| (3,560) | 1:31:A:LYS:HG3 | 1:33:A:HIS:H | 5 | 0.77 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD12 | 7 | 0.77 |
| (3,241) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HE22 | 4 | 0.77 |
| (3,129) | 1:77:A:ILE:HG21 | 1:123:A:ILE:HB | 3 | 0.77 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 3 | 0.77 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 1 | 0.77 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 2 | 0.77 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 9 | 0.77 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 7 | 0.77 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 8 | 0.77 |
| (1,2635) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 10 | 0.77 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 1 | 0.77 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 2 | 0.77 |
| (1,2165) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HA | 1 | 0.77 |
| (1,2165) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HA | 1 | 0.77 |
| (1,2165) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HA | 1 | 0.77 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 1 | 0.77 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 4 | 0.77 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 5 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 5 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 5 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 5 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 7 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 7 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 7 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 10 | 0.77 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 10 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 10 | 0.77 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 2 | 0.77 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 2 | 0.77 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 9 | 0.77 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 9 | 0.77 |
| (1,467) | 1:30:A:GLU:HG2 | 1:30:A:GLU:HA | 9 | 0.77 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 5 | 0.77 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 5 | 0.77 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 6 | 0.76 |
| (3,177) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HA | 4 | 0.76 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB2 | 2 | 0.76 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 5 | 0.76 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 5 | 0.76 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 5 | 0.76 |
| (2,386) | 1:95:A:ASN:HB2 | 1:99:A:PHE:HA | 4 | 0.76 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 9 | 0.76 |
| (1,2849) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 7 | 0.76 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 10 | 0.76 |
| (1,1933) | 1:115:A:VAL:HG21 | 1:116:A:GLU:HA | 4 | 0.76 |
| (1,1933) | 1:115:A:VAL:HG22 | 1:116:A:GLU:HA | 4 | 0.76 |
| (1,1933) | 1:115:A:VAL:HG23 | 1:116:A:GLU:HA | 4 | 0.76 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 9 | 0.76 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 6 | 0.76 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 7 | 0.76 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 7 | 0.76 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 7 | 0.76 |
| (3,1076) | 1:97:A:LYS:H | 1:97:A:LYS:HD3 | 2 | 0.75 |
| (3,401) | 1:15:A:LEU:HD22 | 1:80:A:LEU:HD11 | 4 | 0.75 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB2 | 1 | 0.75 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 10 | 0.75 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 10 | 0.75 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 10 | 0.75 |
| (1,3418) | 1:10:A:ARG:HG3 | 1:9:A:ALA:H | 5 | 0.75 |
| (1,3061) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 5 | 0.75 |
| (1,1933) | 1:115:A:VAL:HG21 | 1:116:A:GLU:HA | 9 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1933) | 1:115:A:VAL:HG22 | 1:116:A:GLU:HA | 9 | 0.75 |
| (1,1933) | 1:115:A:VAL:HG23 | 1:116:A:GLU:HA | 9 | 0.75 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 3 | 0.75 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 3 | 0.75 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 10 | 0.75 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 10 | 0.75 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 10 | 0.75 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 6 | 0.75 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 6 | 0.75 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 6 | 0.75 |
| (1,1886) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD3 | 4 | 0.75 |
| (1,1886) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD3 | 4 | 0.75 |
| (1,1886) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD3 | 4 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 2 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 2 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 2 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 6 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 6 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 6 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 9 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 9 | 0.75 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 9 | 0.75 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 9 | 0.75 |
| (1,1197) | 1:75:A:LYS:HE3 | 1:71:A:PRO:HB2 | 10 | 0.75 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 3 | 0.75 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 7 | 0.75 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 9 | 0.75 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 7 | 0.75 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 7 | 0.75 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 7 | 0.75 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 3 | 0.75 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 5 | 0.75 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 6 | 0.75 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 6 | 0.75 |
| (1,290) | 1:20:A:ILE:HG13 | 1:127:A:ALA:HA | 7 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1155) | 1:118:A:ILE:HG21 | 1:119:A:GLN:H | 2 | 0.74 |
| (3,850) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HH2 | 8 | 0.74 |
| (3,795) | 1:52:A:MET:H | 1:56:A:GLY:HA3 | 3 | 0.74 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 5 | 0.74 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG23 | 6 | 0.74 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG22 | 2 | 0.74 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 6 | 0.74 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 1 | 0.74 |
| (3,379) | 1:45:A:LYS:HA | 1:13:A:TYR:HD1 | 4 | 0.74 |
| (1,3414) | 1:4:A:GLU:H | 1:3:A:GLU:H | 8 | 0.74 |
| (1,3331) | 1:20:A:ILE:H | 1:124:A:SER:HB3 | 6 | 0.74 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 6 | 0.74 |
| (1,2773) | 1:10:A:ARG:HG2 | 1:83:A:GLY:H | 4 | 0.74 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 6 | 0.74 |
| (1,2697) | 1:106:A:GLU:HG2 | 1:90:A:THR:H | 3 | 0.74 |
| (1,2365) | 1:121:A:GLU:H | 1:121:A:GLU:HG2 | 3 | 0.74 |
| (1,2055) | 1:69:A:VAL:H | 1:124:A:SER:HB2 | 3 | 0.74 |
| (1,1933) | 1:115:A:VAL:HG21 | 1:116:A:GLU:HA | 8 | 0.74 |
| (1,1933) | 1:115:A:VAL:HG22 | 1:116:A:GLU:HA | 8 | 0.74 |
| (1,1933) | 1:115:A:VAL:HG23 | 1:116:A:GLU:HA | 8 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 1 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 1 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 1 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 3 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 3 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 3 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 4 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 4 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 4 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 5 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 5 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 5 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 7 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 7 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 7 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 8 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 8 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 8 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG21 | 10 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG22 | 10 | 0.74 |
| (1,1768) | 1:105:A:ILE:HG12 | 1:105:A:ILE:HG23 | 10 | 0.74 |
| (1,1729) | 1:106:A:GLU:HG2 | 1:105:A:ILE:HA | 6 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 1 | 0.74 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 1 | 0.74 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 1 | 0.74 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 1 | 0.74 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 5 | 0.74 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 6 | 0.74 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 6 | 0.74 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 4 | 0.74 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 4 | 0.74 |
| (1,231) | 1:121:A:GLU:H | 1:121:A:GLU:HG2 | 3 | 0.74 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 9 | 0.73 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD13 | 8 | 0.73 |
| (3,850) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HH2 | 2 | 0.73 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG21 | 8 | 0.73 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 5 | 0.73 |
| (3,399) | 1:43:A:ILE:HG23 | 1:44:A:ASP:HA | 7 | 0.73 |
| (3,389) | 1:73:A:PRO:HG3 | 1:91:A:LEU:HD12 | 9 | 0.73 |
| (2,465) | 1:108:A:GLY:H | 1:110:A:LEU:HB3 | 2 | 0.73 |
| (1,3652) | 1:22:A:LYS:H | 1:22:A:LYS:HE2 | 6 | 0.73 |
| (1,3414) | 1:4:A:GLU:H | 1:3:A:GLU:H | 1 | 0.73 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 10 | 0.73 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 7 | 0.73 |
| (1,2636) | 1:96:A:GLU:H | 1:97:A:LYS:HD3 | 10 | 0.73 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG11 | 10 | 0.73 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG12 | 10 | 0.73 |
| (1,2470) | 1:113:A:ARG:H | 1:115:A:VAL:HG13 | 10 | 0.73 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 8 | 0.73 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 1 | 0.73 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 4 | 0.73 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 6 | 0.73 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 7 | 0.73 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 1 | 0.73 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 1 | 0.73 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 1 | 0.73 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 7 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 7 | 0.73 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 7 | 0.73 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 7 | 0.73 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 7 | 0.73 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 7 | 0.73 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 8 | 0.72 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 2 | 0.72 |
| (3,850) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HH2 | 1 | 0.72 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 9 | 0.72 |
| (3,560) | 1:34:A:LYS:HG3 | 1:33:A:HIS:H | 1 | 0.72 |
| (3,366) | 1:16:A:GLN:HG2 | 1:39:A:VAL:HG12 | 5 | 0.72 |
| (1,3061) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 6 | 0.72 |
| (1,2773) | 1:10:A:ARG:HG2 | 1:83:A:GLY:H | 8 | 0.72 |
| (1,2710) | 1:77:A:ILE:HG12 | 1:89:A:GLY:H | 10 | 0.72 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 2 | 0.72 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 5 | 0.72 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 8 | 0.72 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 5 | 0.72 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 10 | 0.72 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 2 | 0.72 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 7 | 0.72 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 10 | 0.72 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 10 | 0.72 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 10 | 0.72 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 2 | 0.72 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 4 | 0.72 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 4 | 0.72 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 4 | 0.72 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 4 | 0.72 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 2 | 0.72 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 2 | 0.72 |
| (3,501) | 1:49:A:VAL:HG11 | 1:40:A:LYS:HB3 | 1 | 0.71 |
| (3,399) | 1:43:A:ILE:HG21 | 1:44:A:ASP:HA | 5 | 0.71 |
| (3,354) | 1:115:A:VAL:H | 1:114:A:ARG:HG3 | 6 | 0.71 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 3 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 6 | 0.71 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 4 | 0.71 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 5 | 0.71 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 8 | 0.71 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 8 | 0.71 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 9 | 0.71 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 5 | 0.71 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 5 | 0.71 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 5 | 0.71 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 7 | 0.71 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 8 | 0.71 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 8 | 0.71 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 8 | 0.71 |
| (3,1139) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 9 | 0.7 |
| (3,1137) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 4 | 0.7 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 5 | 0.7 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG21 | 8 | 0.7 |
| (3,162) | 1:15:A:LEU:H | 1:19:A:ILE:HD11 | 7 | 0.7 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 4 | 0.7 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 4 | 0.7 |
| (1,3501) | 1:40:A:LYS:HE3 | 1:38:A:ILE:H | 5 | 0.7 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 2 | 0.7 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 2 | 0.7 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 2 | 0.7 |
| (1,3331) | 1:20:A:ILE:H | 1:124:A:SER:HB3 | 10 | 0.7 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE1 | 8 | 0.7 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE2 | 8 | 0.7 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 1 | 0.7 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 9 | 0.7 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 8 | 0.7 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 5 | 0.7 |
| (1,2008) | 1:80:A:LEU:HB3 | 1:123:A:ILE:HA | 4 | 0.7 |
| (1,1933) | 1:115:A:VAL:HG21 | 1:116:A:GLU:HA | 6 | 0.7 |
| (1,1933) | 1:115:A:VAL:HG22 | 1:116:A:GLU:HA | 6 | 0.7 |
| (1,1933) | 1:115:A:VAL:HG23 | 1:116:A:GLU:HA | 6 | 0.7 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 9 | 0.7 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 6 | 0.7 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 9 | 0.7 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 5 | 0.7 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 7 | 0.7 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 7 | 0.7 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 7 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 9 | 0.7 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 9 | 0.7 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 9 | 0.7 |
| (3,1140) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 2 | 0.69 |
| (3,1139) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 4 | 0.69 |
| (3,995) | 1:102:A:THR:HG22 | 1:116:A:GLU:H | 5 | 0.69 |
| (3,995) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 9 | 0.69 |
| (3,795) | 1:52:A:MET:H | 1:56:A:GLY:HA3 | 4 | 0.69 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 6 | 0.69 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 10 | 0.69 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG21 | 1 | 0.69 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG21 | 4 | 0.69 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 9 | 0.69 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB2 | 4 | 0.69 |
| (3,162) | 1:15:A:LEU:H | 1:19:A:ILE:HD11 | 9 | 0.69 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 1 | 0.69 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 1 | 0.69 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 1 | 0.69 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 1 | 0.69 |
| (2,46) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HA | 3 | 0.69 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 2 | 0.69 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 3 | 0.69 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 8 | 0.69 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 3 | 0.69 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 3 | 0.69 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 3 | 0.69 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 3 | 0.69 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 1 | 0.69 |
| (1,2357) | 1:122:A:ASP:H | 1:121:A:GLU:HG3 | 3 | 0.69 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 3 | 0.69 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 5 | 0.69 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 5 | 0.69 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 5 | 0.69 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 7 | 0.69 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 9 | 0.69 |
| (1,1954) | 1:118:A:ILE:HD11 | 1:118:A:ILE:HA | 6 | 0.69 |
| (1,1954) | 1:118:A:ILE:HD12 | 1:118:A:ILE:HA | 6 | 0.69 |
| (1,1954) | 1:118:A:ILE:HD13 | 1:118:A:ILE:HA | 6 | 0.69 |
| (1,1529) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 1 | 0.69 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 1 | 0.69 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 1 | 0.69 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 1 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 3 | 0.69 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 3 | 0.69 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 3 | 0.69 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 1 | 0.69 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 2 | 0.69 |
| (1,1177) | 1:70:A:ILE:HG13 | 1:69:A:VAL:HA | 1 | 0.69 |
| (1,896) | 1:51:A:LYS:HE2 | 1:56:A:GLY:HA2 | 5 | 0.69 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 8 | 0.69 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 8 | 0.69 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 2 | 0.69 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 2 | 0.69 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 2 | 0.69 |
| (1,42) | 1:8:A:THR:HA | 1:9:A:ALA:H | 7 | 0.69 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG22 | 6 | 0.68 |
| (3,1036) | 1:21:A:VAL:HG12 | 1:22:A:LYS:H | 6 | 0.68 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 7 | 0.68 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG23 | 1 | 0.68 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG23 | 7 | 0.68 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD13 | 6 | 0.68 |
| (3,501) | 1:49:A:VAL:HG12 | 1:40:A:LYS:HB3 | 9 | 0.68 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD12 | 10 | 0.68 |
| (3,399) | 1:43:A:ILE:HG23 | 1:44:A:ASP:HA | 6 | 0.68 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 8 | 0.68 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 8 | 0.68 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 8 | 0.68 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 5 | 0.68 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG21 | 4 | 0.68 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG22 | 4 | 0.68 |
| (1,2217) | 1:10:A:ARG:HB2 | 1:11:A:THR:HG23 | 4 | 0.68 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 8 | 0.68 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 1 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 2 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 2 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 2 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 6 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 6 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 6 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 7 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 7 | 0.68 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 7 | 0.68 |
| (3,1036) | 1:21:A:VAL:HG11 | 1:22:A:LYS:H | 7 | 0.67 |
| (3,850) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HH2 | 4 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,814) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 6 | 0.67 |
| (3,795) | 1:52:A:MET:H | 1:56:A:GLY:HA3 | 8 | 0.67 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 1 | 0.67 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 2 | 0.67 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 8 | 0.67 |
| (3,339) | 1:30:A:GLU:HG2 | 1:32:A:TYR:H | 2 | 0.67 |
| (3,339) | 1:30:A:GLU:HG2 | 1:32:A:TYR:H | 10 | 0.67 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 1 | 0.67 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 7 | 0.67 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 4 | 0.67 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 4 | 0.67 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 4 | 0.67 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 6 | 0.67 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 6 | 0.67 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 3 | 0.67 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 3 | 0.67 |
| (1,3652) | 1:22:A:LYS:H | 1:22:A:LYS:HE2 | 4 | 0.67 |
| (1,3331) | 1:20:A:ILE:H | 1:124:A:SER:HB3 | 9 | 0.67 |
| (1,3061) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 7 | 0.67 |
| (1,2922) | 1:67:A:GLU:H | 1:22:A:LYS:HB2 | 5 | 0.67 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 7 | 0.67 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 7 | 0.67 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 6 | 0.67 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 7 | 0.67 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 1 | 0.67 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 2 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 8 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 8 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 8 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 9 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 9 | 0.67 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 9 | 0.67 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 9 | 0.67 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 9 | 0.67 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 9 | 0.67 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 4 | 0.67 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 8 | 0.67 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 3 | 0.67 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 4 | 0.67 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 8 | 0.67 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 10 | 0.67 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 5 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 5 | 0.67 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 5 | 0.67 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 5 | 0.67 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 5 | 0.67 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 5 | 0.67 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 3 | 0.67 |
| (3,1181) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 2 | 0.66 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 10 | 0.66 |
| (3,1036) | 1:21:A:VAL:HG13 | 1:22:A:LYS:H | 3 | 0.66 |
| (3,995) | 1:102:A:THR:HG23 | 1:116:A:GLU:H | 4 | 0.66 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 1 | 0.66 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG22 | 5 | 0.66 |
| (3,537) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 10 | 0.66 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 4 | 0.66 |
| (3,300) | 1:11:A:THR:HG23 | 1:13:A:TYR:HE2 | 6 | 0.66 |
| (1,3726) | 1:95:A:ASN:HD21 | 1:98:A:THR:HB | 9 | 0.66 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 7 | 0.66 |
| (1,3469) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE21 | 6 | 0.66 |
| (1,3469) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE21 | 6 | 0.66 |
| (1,3469) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE21 | 6 | 0.66 |
| (1,3434) | 1:63:A:GLN:HE22 | 1:14:A:TRP:HE1 | 3 | 0.66 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 6 | 0.66 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 6 | 0.66 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 6 | 0.66 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 7 | 0.66 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 6 | 0.66 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 9 | 0.66 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 4 | 0.66 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 7 | 0.66 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 5 | 0.66 |
| (1,1488) | 1:106:A:GLU:HG2 | 1:89:A:GLY:HA2 | 6 | 0.66 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 6 | 0.66 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 6 | 0.66 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 6 | 0.66 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 6 | 0.66 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 3 | 0.66 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 3 | 0.66 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 3 | 0.66 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 9 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 9 | 0.66 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 10 | 0.66 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 10 | 0.66 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 5 | 0.66 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 5 | 0.66 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 10 | 0.66 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 10 | 0.66 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 10 | 0.66 |
| (1,42) | 1:8:A:THR:HA | 1:9:A:ALA:H | 3 | 0.66 |
| (3,1036) | 1:21:A:VAL:HG13 | 1:22:A:LYS:H | 1 | 0.65 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 2 | 0.65 |
| (2,46) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HA | 5 | 0.65 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 9 | 0.65 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 9 | 0.65 |
| (1,3594) | 1:97:A:LYS:H | 1:95:A:ASN:HD22 | 5 | 0.65 |
| (1,3591) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD21 | 9 | 0.65 |
| (1,3591) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD21 | 9 | 0.65 |
| (1,3591) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD21 | 9 | 0.65 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 8 | 0.65 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 9 | 0.65 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 5 | 0.65 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 2 | 0.65 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 10 | 0.65 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 10 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 10 | 0.65 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 8 | 0.65 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 9 | 0.65 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 6 | 0.65 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 6 | 0.65 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 6 | 0.65 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 8 | 0.65 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 8 | 0.65 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 8 | 0.65 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 1 | 0.65 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 1 | 0.65 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 10 | 0.65 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 10 | 0.65 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 10 | 0.65 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 3 | 0.65 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 3 | 0.65 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 3 | 0.65 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 6 | 0.65 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 5 | 0.65 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 6 | 0.65 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 6 | 0.65 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 6 | 0.65 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 6 | 0.65 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 6 | 0.65 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 6 | 0.65 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 10 | 0.65 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 5 | 0.65 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 5 | 0.65 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 5 | 0.65 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 5 | 0.65 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 6 | 0.65 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 3 | 0.65 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 3 | 0.65 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 1 | 0.65 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 1 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 1 | 0.65 |
| (3,1155) | 1:118:A:ILE:HG21 | 1:119:A:GLN:H | 3 | 0.64 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG22 | 7 | 0.64 |
| (3,1036) | 1:21:A:VAL:HG13 | 1:22:A:LYS:H | 8 | 0.64 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 8 | 0.64 |
| (3,582) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 4 | 0.64 |
| (3,32) | 1:22:A:LYS:HD2 | 1:34:A:LYS:HA | 2 | 0.64 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 6 | 0.64 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 6 | 0.64 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 6 | 0.64 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 7 | 0.64 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 7 | 0.64 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 7 | 0.64 |
| (1,2880) | 1:75:A:LYS:HB3 | 1:72:A:ALA:H | 10 | 0.64 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 5 | 0.64 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 9 | 0.64 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 10 | 0.64 |
| (1,2475) | 1:110:A:LEU:HD11 | 1:111:A:LYS:H | 10 | 0.64 |
| (1,2475) | 1:110:A:LEU:HD12 | 1:111:A:LYS:H | 10 | 0.64 |
| (1,2475) | 1:110:A:LEU:HD13 | 1:111:A:LYS:H | 10 | 0.64 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 3 | 0.64 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 3 | 0.64 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 3 | 0.64 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 3 | 0.64 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 2 | 0.64 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 3 | 0.64 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 7 | 0.64 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 7 | 0.64 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 4 | 0.64 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 8 | 0.64 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 9 | 0.64 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 4 | 0.64 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 4 | 0.64 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 4 | 0.64 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 1 | 0.64 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 3 | 0.64 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 8 | 0.64 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 8 | 0.64 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 8 | 0.64 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 7 | 0.64 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 8 | 0.64 |
| (3,1157) | 1:80:A:LEU:HD11 | 1:14:A:TRP:HZ3 | 1 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1157) | 1:80:A:LEU:HD11 | 1:14:A:TRP:HZ3 | 9 | 0.63 |
| (3,1068) | 1:126:A:LEU:H | 1:76:A:ARG:HB2 | 1 | 0.63 |
| (3,975) | 1:97:A:LYS:HB2 | 1:98:A:THR:HG21 | 4 | 0.63 |
| (3,850) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HH2 | 7 | 0.63 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG22 | 2 | 0.63 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG21 | 3 | 0.63 |
| (3,699) | 1:110:A:LEU:HA | 1:105:A:ILE:HG22 | 9 | 0.63 |
| (3,582) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 9 | 0.63 |
| (3,518) | 1:26:A:LYS:HD2 | 1:30:A:GLU:HG2 | 6 | 0.63 |
| (3,354) | 1:115:A:VAL:H | 1:118:A:ILE:HG13 | 4 | 0.63 |
| (3,32) | 1:34:A:LYS:HA | 1:34:A:LYS:HD2 | 6 | 0.63 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD11 | 1 | 0.63 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 4 | 0.63 |
| (2,142) | 1:10:A:ARG:HA | 1:82:A:GLY:HA3 | 2 | 0.63 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 2 | 0.63 |
| (1,2850) | 1:75:A:LYS:HB3 | 1:76:A:ARG:H | 10 | 0.63 |
| (1,2734) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 1 | 0.63 |
| (1,2406) | 1:118:A:ILE:HD11 | 1:119:A:GLN:H | 6 | 0.63 |
| (1,2406) | 1:118:A:ILE:HD12 | 1:119:A:GLN:H | 6 | 0.63 |
| (1,2406) | 1:118:A:ILE:HD13 | 1:119:A:GLN:H | 6 | 0.63 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 6 | 0.63 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 2 | 0.63 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 2 | 0.63 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 2 | 0.63 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 8 | 0.63 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 8 | 0.63 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD21 | 2 | 0.63 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD22 | 2 | 0.63 |
| (1,1285) | 1:76:A:ARG:HG2 | 1:126:A:LEU:HD23 | 2 | 0.63 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 3 | 0.63 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 10 | 0.63 |
| (1,1096) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HB3 | 10 | 0.63 |
| (1,1096) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HB3 | 10 | 0.63 |
| (1,1096) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HB3 | 10 | 0.63 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 4 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 4 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 6 | 0.63 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 6 | 0.63 |
| (3,1036) | 1:21:A:VAL:HG11 | 1:22:A:LYS:H | 9 | 0.62 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG23 | 10 | 0.62 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 7 | 0.62 |
| (3,475) | 1:32:A:TYR:HB2 | 1:30:A:GLU:HA | 2 | 0.62 |
| (3,449) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG23 | 10 | 0.62 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB1 | 6 | 0.62 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 7 | 0.62 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 7 | 0.62 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 7 | 0.62 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 4 | 0.62 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 5 | 0.62 |
| (1,3522) | 1:40:A:LYS:HE3 | 1:51:A:LYS:H | 5 | 0.62 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 8 | 0.62 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 8 | 0.62 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 8 | 0.62 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 9 | 0.62 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 6 | 0.62 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 4 | 0.62 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 5 | 0.62 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 5 | 0.62 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 5 | 0.62 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 10 | 0.62 |
| (1,1928) | 1:115:A:VAL:HG21 | 1:84:A:TYR:HD1 | 5 | 0.62 |
| (1,1928) | 1:115:A:VAL:HG21 | 1:84:A:TYR:HD2 | 5 | 0.62 |
| (1,1928) | 1:115:A:VAL:HG22 | 1:84:A:TYR:HD1 | 5 | 0.62 |
| (1,1928) | 1:115:A:VAL:HG22 | 1:84:A:TYR:HD2 | 5 | 0.62 |
| (1,1928) | 1:115:A:VAL:HG23 | 1:84:A:TYR:HD1 | 5 | 0.62 |
| (1,1928) | 1:115:A:VAL:HG23 | 1:84:A:TYR:HD2 | 5 | 0.62 |
| (1,1869) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 9 | 0.62 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 8 | 0.62 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 5 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 5 | 0.62 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 5 | 0.62 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 7 | 0.62 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 7 | 0.62 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 7 | 0.62 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 5 | 0.62 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 3 | 0.62 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 4 | 0.62 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 4 | 0.62 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 4 | 0.62 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 8 | 0.62 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 8 | 0.62 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 8 | 0.62 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 8 | 0.62 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 8 | 0.62 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 8 | 0.62 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 8 | 0.62 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 9 | 0.62 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 7 | 0.62 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 9 | 0.62 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 7 | 0.62 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 7 | 0.62 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 7 | 0.62 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 6 | 0.62 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 6 | 0.62 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 6 | 0.62 |
| (3,1095) | 1:27:A:LYS:HB3 | 1:25:A:THR:H | 6 | 0.61 |
| (3,399) | 1:43:A:ILE:HG22 | 1:44:A:ASP:HA | 1 | 0.61 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 2 | 0.61 |
| (3,165) | 1:79:A:VAL:HG12 | 1:88:A:GLU:HA | 4 | 0.61 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD11 | 7 | 0.61 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 3 | 0.61 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 3 | 0.61 |
| (1,3714) | 1:84:A:TYR:HD1 | 1:87:A:ASN:HD22 | 4 | 0.61 |
| (1,3714) | 1:84:A:TYR:HD2 | 1:87:A:ASN:HD22 | 4 | 0.61 |
| (1,3694) | 1:68:A:THR:H | 1:22:A:LYS:HB2 | 2 | 0.61 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG21 | 3 | 0.61 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG22 | 3 | 0.61 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG23 | 3 | 0.61 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 1 | 0.61 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 4 | 0.61 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 9 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2685) | 1:76:A:ARG:HD2 | 1:91:A:LEU:H | 5 | 0.61 |
| (1,2434) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 3 | 0.61 |
| (1,2305) | 1:104:A:VAL:HG11 | 1:114:A:ARG:HG2 | 4 | 0.61 |
| (1,2305) | 1:104:A:VAL:HG12 | 1:114:A:ARG:HG2 | 4 | 0.61 |
| (1,2305) | 1:104:A:VAL:HG13 | 1:114:A:ARG:HG2 | 4 | 0.61 |
| (1,2222) | 1:117:A:GLY:H | 1:100:A:SER:HB3 | 3 | 0.61 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 1 | 0.61 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 1 | 0.61 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 1 | 0.61 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 9 | 0.61 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 4 | 0.61 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 4 | 0.61 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 4 | 0.61 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 4 | 0.61 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 1 | 0.61 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 2 | 0.61 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 8 | 0.61 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 8 | 0.61 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 8 | 0.61 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 10 | 0.61 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 10 | 0.61 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 10 | 0.61 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 1 | 0.61 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 4 | 0.61 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 10 | 0.61 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 7 | 0.61 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 7 | 0.61 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 7 | 0.61 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD12 | 6 | 0.6 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 9 | 0.6 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 3 | 0.6 |
| (3,339) | 1:30:A:GLU:HG2 | 1:32:A:TYR:H | 3 | 0.6 |
| (3,162) | 1:15:A:LEU:H | 1:48:A:ALA:HB3 | 3 | 0.6 |
| (3,122) | 1:40:A:LYS:HE2 | 1:38:A:ILE:HG23 | 3 | 0.6 |
| (2,650) | 1:61:A:LEU:HB2 | 1:65:A:HIS:HD2 | 8 | 0.6 |
| (2,589) | 1:82:A:GLY:HA3 | 1:11:A:THR:H | 3 | 0.6 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 7 | 0.6 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 4 | 0.6 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 9 | 0.6 |
| (1,3509) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 5 | 0.6 |
| (1,3403) | 1:10:A:ARG:HD2 | 1:10:A:ARG:H | 7 | 0.6 |
| (1,2591) | 1:95:A:ASN:HB2 | 1:100:A:SER:H | 2 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 3 | 0.6 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 3 | 0.6 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 4 | 0.6 |
| (1,2333) | 1:125:A:LYS:H | 1:71:A:PRO:HD2 | 7 | 0.6 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 6 | 0.6 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 6 | 0.6 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 6 | 0.6 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 10 | 0.6 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 10 | 0.6 |
| (1,1880) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 10 | 0.6 |
| (1,1606) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 8 | 0.6 |
| (1,1606) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 9 | 0.6 |
| (1,1606) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 10 | 0.6 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 9 | 0.6 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 3 | 0.6 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 2 | 0.6 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 2 | 0.6 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 2 | 0.6 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 4 | 0.6 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 7 | 0.6 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 3 | 0.6 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 4 | 0.6 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 4 | 0.6 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 4 | 0.6 |
| (1,1097) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HB3 | 10 | 0.6 |
| (1,1097) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HB3 | 10 | 0.6 |
| (1,1097) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HB3 | 10 | 0.6 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 2 | 0.6 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 2 | 0.6 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 2 | 0.6 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 9 | 0.6 |
| (1,817) | 1:51:A:LYS:HG3 | 1:56:A:GLY:HA3 | 1 | 0.6 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 2 | 0.6 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 2 | 0.6 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 3 | 0.6 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 3 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 3 | 0.6 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 7 | 0.6 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 7 | 0.6 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 7 | 0.6 |
| (1,441) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HA | 3 | 0.6 |
| (1,441) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HA | 3 | 0.6 |
| (1,441) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HA | 3 | 0.6 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 3 | 0.6 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 1 | 0.6 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 2 | 0.6 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 6 | 0.59 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 5 | 0.59 |
| (3,1157) | 1:80:A:LEU:HD13 | 1:14:A:TRP:HZ3 | 3 | 0.59 |
| (3,1137) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 6 | 0.59 |
| (3,1036) | 1:21:A:VAL:HG12 | 1:22:A:LYS:H | 10 | 0.59 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG23 | 5 | 0.59 |
| (3,449) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 6 | 0.59 |
| (3,300) | 1:11:A:THR:HG22 | 1:13:A:TYR:HE1 | 9 | 0.59 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 8 | 0.59 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 2 | 0.59 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 2 | 0.59 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 4 | 0.59 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 4 | 0.59 |
| (1,3758) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 2 | 0.59 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 6 | 0.59 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 6 | 0.59 |
| (1,3346) | 1:39:A:VAL:HG21 | 1:18:A:GLU:H | 9 | 0.59 |
| (1,3346) | 1:39:A:VAL:HG22 | 1:18:A:GLU:H | 9 | 0.59 |
| (1,3346) | 1:39:A:VAL:HG23 | 1:18:A:GLU:H | 9 | 0.59 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 3 | 0.59 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 6 | 0.59 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 8 | 0.59 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 10 | 0.59 |
| (1,2792) | 1:81:A:ASN:H | 1:81:A:ASN:HB3 | 9 | 0.59 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 10 | 0.59 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 6 | 0.59 |
| (1,2536) | 1:106:A:GLU:HG2 | 1:104:A:VAL:H | 6 | 0.59 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 9 | 0.59 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 3 | 0.59 |
| (1,2162) | 1:115:A:VAL:HG21 | 1:113:A:ARG:HD3 | 7 | 0.59 |
| (1,2162) | 1:115:A:VAL:HG22 | 1:113:A:ARG:HD3 | 7 | 0.59 |
| (1,2162) | 1:115:A:VAL:HG23 | 1:113:A:ARG:HD3 | 7 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 1 | 0.59 |
| (1,1881) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 10 | 0.59 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG11 | 7 | 0.59 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG12 | 7 | 0.59 |
| (1,1873) | 1:113:A:ARG:HB2 | 1:115:A:VAL:HG13 | 7 | 0.59 |
| (1,1606) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 3 | 0.59 |
| (1,1606) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 4 | 0.59 |
| (1,1606) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 5 | 0.59 |
| (1,1606) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 7 | 0.59 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 5 | 0.59 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 9 | 0.59 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 4 | 0.59 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 4 | 0.59 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 4 | 0.59 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 9 | 0.59 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 9 | 0.59 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 9 | 0.59 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 8 | 0.59 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 3 | 0.59 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 3 | 0.59 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 3 | 0.59 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 5 | 0.59 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 5 | 0.59 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 1 | 0.59 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 6 | 0.59 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 2 | 0.59 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 2 | 0.59 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 2 | 0.59 |
| (1,165) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HG2 | 6 | 0.59 |
| (1,165) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HG2 | 6 | 0.59 |
| (1,165) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HG2 | 6 | 0.59 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 5 | 0.59 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 9 | 0.58 |
| (3,900) | 1:34:A:LYS:HE3 | 1:34:A:LYS:HG3 | 1 | 0.58 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD13 | 9 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,850) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HH2 | 9 | 0.58 |
| (3,849) | 1:35:A:LYS:HD2 | 1:33:A:HIS:H | 6 | 0.58 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD12 | 4 | 0.58 |
| (3,449) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 1 | 0.58 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG22 | 2 | 0.58 |
| (3,449) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG23 | 4 | 0.58 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG21 | 7 | 0.58 |
| (3,449) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG22 | 8 | 0.58 |
| (3,423) | 1:61:A:LEU:HD13 | 1:25:A:THR:H | 2 | 0.58 |
| (3,300) | 1:11:A:THR:HG22 | 1:13:A:TYR:HE1 | 10 | 0.58 |
| (3,241) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HE22 | 6 | 0.58 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 4 | 0.58 |
| (1,3753) | 1:34:A:LYS:HD2 | 1:33:A:HIS:HE1 | 10 | 0.58 |
| (1,3714) | 1:84:A:TYR:HD1 | 1:87:A:ASN:HD22 | 6 | 0.58 |
| (1,3714) | 1:84:A:TYR:HD2 | 1:87:A:ASN:HD22 | 6 | 0.58 |
| (1,3656) | 1:32:A:TYR:HB2 | 1:27:A:LYS:H | 6 | 0.58 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 5 | 0.58 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 8 | 0.58 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 10 | 0.58 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 10 | 0.58 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 10 | 0.58 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE3 | 6 | 0.58 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 10 | 0.58 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 8 | 0.58 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 2 | 0.58 |
| (1,2666) | 1:93:A:SER:H | 1:91:A:LEU:HG | 6 | 0.58 |
| (1,2591) | 1:95:A:ASN:HB2 | 1:100:A:SER:H | 1 | 0.58 |
| (1,2536) | 1:106:A:GLU:HG2 | 1:104:A:VAL:H | 3 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 1 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 1 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 1 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 2 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 2 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 2 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 3 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 3 | 0.58 |
| (1,1919) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 3 | 0.58 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 3 | 0.58 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 3 | 0.58 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 3 | 0.58 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 3 | 0.58 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 3 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 3 | 0.58 |
| (1,1478) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HB3 | 4 | 0.58 |
| (1,1478) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HB3 | 4 | 0.58 |
| (1,1478) | 1:126:A:LEU:HD23 | 1:88:A:GLU:HB3 | 4 | 0.58 |
| (1,1273) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 10 | 0.58 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 9 | 0.58 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 7 | 0.58 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 2 | 0.58 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 2 | 0.58 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 2 | 0.58 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 6 | 0.58 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 6 | 0.58 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 6 | 0.58 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD11 | 1 | 0.58 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD12 | 1 | 0.58 |
| (1,685) | 1:60:A:LYS:HE3 | 1:43:A:ILE:HD13 | 1 | 0.58 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 7 | 0.58 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 7 | 0.58 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 5 | 0.57 |
| (3,1155) | 1:118:A:ILE:HG23 | 1:119:A:GLN:H | 1 | 0.57 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD11 | 8 | 0.57 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 4 | 0.57 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 7 | 0.57 |
| (3,449) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 3 | 0.57 |
| (3,449) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG22 | 9 | 0.57 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 5 | 0.57 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG21 | 1 | 0.57 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 6 | 0.57 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 6 | 0.57 |
| (1,3560) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 10 | 0.57 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 5 | 0.57 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 5 | 0.57 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 5 | 0.57 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 8 | 0.57 |
| (1,3112) | 1:46:A:TYR:HB3 | 1:46:A:TYR:H | 10 | 0.57 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 2 | 0.57 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 8 | 0.57 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 4 | 0.57 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 5 | 0.57 |
| (1,2450) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 10 | 0.57 |
| (1,2450) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 10 | 0.57 |
| (1,2450) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 10 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2157) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB3 | 3 | 0.57 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 8 | 0.57 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 8 | 0.57 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 8 | 0.57 |
| (1,1919) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 5 | 0.57 |
| (1,1919) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 5 | 0.57 |
| (1,1919) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 5 | 0.57 |
| (1,1919) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 7 | 0.57 |
| (1,1919) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 7 | 0.57 |
| (1,1919) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 7 | 0.57 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 3 | 0.57 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 3 | 0.57 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 3 | 0.57 |
| (1,1265) | 1:76:A:ARG:H | 1:76:A:ARG:HG3 | 7 | 0.57 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 5 | 0.57 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 5 | 0.57 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 5 | 0.57 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 1 | 0.57 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 1 | 0.57 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 1 | 0.57 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 1 | 0.57 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 1 | 0.57 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 1 | 0.57 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 2 | 0.57 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 6 | 0.57 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 6 | 0.57 |
| (1,477) | 1:31:A:LYS:HB2 | 1:31:A:LYS:HA | 1 | 0.57 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 2 | 0.57 |
| (1,330) | 1:31:A:LYS:HE3 | 1:31:A:LYS:HG3 | 10 | 0.57 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 3 | 0.57 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HG2 | 2 | 0.56 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 9 | 0.56 |
| (3,1093) | 1:70:A:ILE:HD11 | 1:123:A:ILE:H | 9 | 0.56 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 3 | 0.56 |
| (3,1036) | 1:21:A:VAL:HG12 | 1:22:A:LYS:H | 2 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1036) | 1:21:A:VAL:HG11 | 1:22:A:LYS:H | 5 | 0.56 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 5 | 0.56 |
| (3,857) | 1:114:A:ARG:HB3 | 1:115:A:VAL:HG11 | 10 | 0.56 |
| (3,603) | 1:25:A:THR:HG22 | 1:23:A:ILE:HD13 | 1 | 0.56 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 3 | 0.56 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 6 | 0.56 |
| (3,414) | 1:22:A:LYS:HD2 | 1:34:A:LYS:HA | 2 | 0.56 |
| (3,414) | 1:34:A:LYS:HA | 1:34:A:LYS:HD2 | 6 | 0.56 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 5 | 0.56 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 6 | 0.56 |
| (3,399) | 1:43:A:ILE:HG22 | 1:44:A:ASP:HA | 3 | 0.56 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 9 | 0.56 |
| (3,32) | 1:22:A:LYS:HD2 | 1:34:A:LYS:HA | 4 | 0.56 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 6 | 0.56 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 6 | 0.56 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 6 | 0.56 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 10 | 0.56 |
| (1,3443) | 1:63:A:GLN:HG3 | 1:14:A:TRP:HE1 | 6 | 0.56 |
| (1,3421) | 1:10:A:ARG:H | 1:82:A:GLY:HA3 | 8 | 0.56 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 5 | 0.56 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 3 | 0.56 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 8 | 0.56 |
| (1,2450) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 4 | 0.56 |
| (1,2450) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 4 | 0.56 |
| (1,2450) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 4 | 0.56 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 10 | 0.56 |
| (1,2223) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 2 | 0.56 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 9 | 0.56 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 9 | 0.56 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 9 | 0.56 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 9 | 0.56 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 9 | 0.56 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 9 | 0.56 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 1 | 0.56 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 4 | 0.56 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 5 | 0.56 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 5 | 0.56 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 5 | 0.56 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 5 | 0.56 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 5 | 0.56 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 5 | 0.56 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 3 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 4 | 0.56 |
| (1,834) | 1:52:A:MET:HG2 | 1:59:A:LEU:HG | 9 | 0.56 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 1 | 0.56 |
| (1,477) | 1:31:A:LYS:HB2 | 1:31:A:LYS:HA | 5 | 0.56 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 6 | 0.56 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 6 | 0.56 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 6 | 0.56 |
| (1,210) | 1:18:A:GLU:HA | 1:18:A:GLU:HG2 | 4 | 0.56 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 1 | 0.56 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 1 | 0.56 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 1 | 0.56 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 3 | 0.56 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 3 | 0.56 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 3 | 0.56 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 6 | 0.56 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 6 | 0.56 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 6 | 0.56 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 8 | 0.56 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 8 | 0.56 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 8 | 0.56 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 10 | 0.56 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 10 | 0.56 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 10 | 0.56 |
| (1,42) | 1:8:A:THR:HA | 1:9:A:ALA:H | 9 | 0.56 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:110:A:LEU:HB2 | 9 | 0.55 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 7 | 0.55 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 10 | 0.55 |
| (3,1144) | 1:45:A:LYS:H | 1:45:A:LYS:HD2 | 2 | 0.55 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 2 | 0.55 |
| (3,1093) | 1:70:A:ILE:HD11 | 1:123:A:ILE:H | 2 | 0.55 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD13 | 4 | 0.55 |
| (3,777) | 1:18:A:GLU:H | 1:38:A:ILE:HG23 | 3 | 0.55 |
| (3,582) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 2 | 0.55 |
| (3,399) | 1:43:A:ILE:HG21 | 1:44:A:ASP:HA | 10 | 0.55 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 8 | 0.55 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 3 | 0.55 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 2 | 0.55 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 2 | 0.55 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 2 | 0.55 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE2 | 2 | 0.55 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 3 | 0.55 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 9 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 2 | 0.55 |
| (1,2751) | 1:78:A:LEU:HD21 | 1:86:A:GLY:H | 6 | 0.55 |
| (1,2751) | 1:78:A:LEU:HD22 | 1:86:A:GLY:H | 6 | 0.55 |
| (1,2751) | 1:78:A:LEU:HD23 | 1:86:A:GLY:H | 6 | 0.55 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 4 | 0.55 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 1 | 0.55 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 1 | 0.55 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 1 | 0.55 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 6 | 0.55 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 6 | 0.55 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 6 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 6 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 6 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 6 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 8 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 8 | 0.55 |
| (1,2450) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 8 | 0.55 |
| (1,2158) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 4 | 0.55 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 9 | 0.55 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 9 | 0.55 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 6 | 0.55 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 6 | 0.55 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 6 | 0.55 |
| (1,1481) | 1:88:A:GLU:HG3 | 1:88:A:GLU:H | 1 | 0.55 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 5 | 0.55 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 2 | 0.55 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 4 | 0.55 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 4 | 0.55 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 4 | 0.55 |
| (1,751) | 1:46:A:TYR:HA | 1:63:A:GLN:HB2 | 8 | 0.55 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 10 | 0.55 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 5 | 0.55 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 6 | 0.55 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 6 | 0.55 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 7 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 7 | 0.55 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 7 | 0.55 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 8 | 0.55 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 8 | 0.55 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 8 | 0.55 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 9 | 0.55 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 9 | 0.55 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 9 | 0.55 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 1 | 0.55 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 1 | 0.55 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 1 | 0.55 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 3 | 0.55 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 3 | 0.55 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 3 | 0.55 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 6 | 0.55 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 6 | 0.55 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 6 | 0.55 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 8 | 0.55 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 8 | 0.55 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 8 | 0.55 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 10 | 0.55 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 10 | 0.55 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 10 | 0.55 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 2 | 0.55 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 2 | 0.55 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 2 | 0.55 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 4 | 0.55 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 4 | 0.55 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 4 | 0.55 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 7 | 0.55 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 7 | 0.55 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 7 | 0.55 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 8 | 0.55 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 4 | 0.55 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 6 | 0.55 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 9 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 10 | 0.55 |
| (3,1183) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 2 | 0.54 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 4 | 0.54 |
| (3,1049) | 1:109:A:PRO:HA | 1:109:A:PRO:HG2 | 5 | 0.54 |
| (3,975) | 1:77:A:ILE:HB | 1:123:A:ILE:HG21 | 6 | 0.54 |
| (3,941) | 1:12:A:ASP:HA | 1:12:A:ASP:HB3 | 10 | 0.54 |
| (3,878) | 1:14:A:TRP:H | 1:14:A:TRP:HE1 | 8 | 0.54 |
| (3,841) | 1:80:A:LEU:HD23 | 1:80:A:LEU:H | 7 | 0.54 |
| (3,800) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 4 | 0.54 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 3 | 0.54 |
| (3,401) | 1:15:A:LEU:HD23 | 1:80:A:LEU:HD13 | 5 | 0.54 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 1 | 0.54 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 7 | 0.54 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 3 | 0.54 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 9 | 0.54 |
| (3,305) | 1:118:A:ILE:HG13 | 1:103:A:ILE:HG13 | 6 | 0.54 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 4 | 0.54 |
| (2,142) | 1:10:A:ARG:HA | 1:82:A:GLY:HA3 | 6 | 0.54 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 5 | 0.54 |
| (1,3648) | 1:16:A:GLN:HE22 | 1:80:A:LEU:HG | 5 | 0.54 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 1 | 0.54 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 3 | 0.54 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 7 | 0.54 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 4 | 0.54 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 4 | 0.54 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 4 | 0.54 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 7 | 0.54 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 5 | 0.54 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 6 | 0.54 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 3 | 0.54 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 9 | 0.54 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 9 | 0.54 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 9 | 0.54 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 10 | 0.54 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 10 | 0.54 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 10 | 0.54 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 4 | 0.54 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 7 | 0.54 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 2 | 0.54 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 2 | 0.54 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 2 | 0.54 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 2 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 3 | 0.54 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 1 | 0.54 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 1 | 0.54 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 1 | 0.54 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 2 | 0.54 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 2 | 0.54 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 2 | 0.54 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 2 | 0.54 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 5 | 0.54 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 6 | 0.54 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 1 | 0.54 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 2 | 0.54 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 4 | 0.54 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 9 | 0.54 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 10 | 0.54 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 1 | 0.54 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 4 | 0.54 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 4 | 0.54 |
| (1,441) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HA | 9 | 0.54 |
| (1,441) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HA | 9 | 0.54 |
| (1,441) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HA | 9 | 0.54 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 6 | 0.54 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 6 | 0.54 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 6 | 0.54 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 2 | 0.54 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 2 | 0.54 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 2 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 4 | 0.54 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 4 | 0.54 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 4 | 0.54 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 7 | 0.54 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 7 | 0.54 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 7 | 0.54 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 2 | 0.54 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 2 | 0.54 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 2 | 0.54 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 5 | 0.54 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 5 | 0.54 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 5 | 0.54 |
| (1,115) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 9 | 0.54 |
| (1,115) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 9 | 0.54 |
| (1,115) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 9 | 0.54 |
| (1,33) | 1:113:A:ARG:HA | 1:113:A:ARG:HG3 | 8 | 0.54 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG23 | 1 | 0.53 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG23 | 10 | 0.53 |
| (3,1049) | 1:109:A:PRO:HA | 1:109:A:PRO:HG2 | 10 | 0.53 |
| (3,961) | 1:30:A:GLU:HG2 | 1:29:A:GLY:H | 8 | 0.53 |
| (3,849) | 1:26:A:LYS:HB3 | 1:33:A:HIS:H | 5 | 0.53 |
| (3,849) | 1:26:A:LYS:HB3 | 1:33:A:HIS:H | 7 | 0.53 |
| (3,795) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 1 | 0.53 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 5 | 0.53 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 10 | 0.53 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 9 | 0.53 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 7 | 0.53 |
| (3,366) | 1:42:A:VAL:HG23 | 1:16:A:GLN:HG2 | 3 | 0.53 |
| (3,21) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HG2 | 1 | 0.53 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 10 | 0.53 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD11 | 6 | 0.53 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD12 | 6 | 0.53 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD13 | 6 | 0.53 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD11 | 6 | 0.53 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD12 | 6 | 0.53 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD13 | 6 | 0.53 |
| (1,3758) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 5 | 0.53 |
| (1,3715) | 1:84:A:TYR:HE1 | 1:87:A:ASN:HD22 | 6 | 0.53 |
| (1,3715) | 1:84:A:TYR:HE2 | 1:87:A:ASN:HD22 | 6 | 0.53 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 6 | 0.53 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG21 | 4 | 0.53 |
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG22 | 4 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3399) | 1:11:A:THR:H | 1:11:A:THR:HG23 | 4 | 0.53 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 8 | 0.53 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 8 | 0.53 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 8 | 0.53 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 8 | 0.53 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 1 | 0.53 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 6 | 0.53 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 3 | 0.53 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 6 | 0.53 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 8 | 0.53 |
| (1,2450) | 1:115:A:VAL:HG11 | 1:115:A:VAL:H | 9 | 0.53 |
| (1,2450) | 1:115:A:VAL:HG12 | 1:115:A:VAL:H | 9 | 0.53 |
| (1,2450) | 1:115:A:VAL:HG13 | 1:115:A:VAL:H | 9 | 0.53 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 1 | 0.53 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 7 | 0.53 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 7 | 0.53 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 7 | 0.53 |
| (1,2158) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 7 | 0.53 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 5 | 0.53 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 9 | 0.53 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 10 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 6 | 0.53 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 6 | 0.53 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 1 | 0.53 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 1 | 0.53 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 1 | 0.53 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 1 | 0.53 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 1 | 0.53 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 1 | 0.53 |
| (1,1541) | 1:93:A:SER:H | 1:92:A:GLU:HG3 | 8 | 0.53 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD11 | 9 | 0.53 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD12 | 9 | 0.53 |
| (1,1521) | 1:73:A:PRO:HD2 | 1:91:A:LEU:HD13 | 9 | 0.53 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 2 | 0.53 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 2 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 2 | 0.53 |
| (1,1274) | 1:77:A:ILE:HG12 | 1:76:A:ARG:HA | 10 | 0.53 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 4 | 0.53 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 4 | 0.53 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 4 | 0.53 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 3 | 0.53 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 3 | 0.53 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 3 | 0.53 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 3 | 0.53 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 7 | 0.53 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 5 | 0.53 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 3 | 0.53 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 6 | 0.53 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 2 | 0.53 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 2 | 0.53 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 2 | 0.53 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 3 | 0.53 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 3 | 0.53 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 3 | 0.53 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 3 | 0.53 |
| (1,397) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 5 | 0.53 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 4 | 0.53 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 4 | 0.53 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 4 | 0.53 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 5 | 0.53 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 5 | 0.53 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 5 | 0.53 |
| (1,142) | 1:15:A:LEU:HD11 | 1:15:A:LEU:HA | 9 | 0.53 |
| (1,142) | 1:15:A:LEU:HD12 | 1:15:A:LEU:HA | 9 | 0.53 |
| (1,142) | 1:15:A:LEU:HD13 | 1:15:A:LEU:HA | 9 | 0.53 |
| (1,42) | 1:8:A:THR:HA | 1:9:A:ALA:H | 10 | 0.53 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 1 | 0.52 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 8 | 0.52 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 5 | 0.52 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 10 | 0.52 |
| (3,1093) | 1:70:A:ILE:HD13 | 1:123:A:ILE:H | 7 | 0.52 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 1 | 0.52 |
| (3,1036) | 1:21:A:VAL:HG12 | 1:22:A:LYS:H | 4 | 0.52 |
| (3,841) | 1:80:A:LEU:HD21 | 1:80:A:LEU:H | 2 | 0.52 |
| (3,814) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 10 | 0.52 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 10 | 0.52 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 7 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,603) | 1:25:A:THR:HG23 | 1:23:A:ILE:HD13 | 10 | 0.52 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG22 | 9 | 0.52 |
| (3,416) | 1:5:A:LYS:H | 1:4:A:GLU:HG2 | 9 | 0.52 |
| (3,397) | 1:40:A:LYS:HE2 | 1:40:A:LYS:HA | 10 | 0.52 |
| (3,391) | 1:114:A:ARG:H | 1:114:A:ARG:HG3 | 3 | 0.52 |
| (3,339) | 1:30:A:GLU:HG3 | 1:32:A:TYR:H | 4 | 0.52 |
| (3,240) | 1:109:A:PRO:HA | 1:109:A:PRO:HG2 | 5 | 0.52 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 8 | 0.52 |
| (1,3715) | 1:84:A:TYR:HE1 | 1:87:A:ASN:HD22 | 4 | 0.52 |
| (1,3715) | 1:84:A:TYR:HE2 | 1:87:A:ASN:HD22 | 4 | 0.52 |
| (1,3556) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 2 | 0.52 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 3 | 0.52 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 10 | 0.52 |
| (1,3449) | 1:15:A:LEU:H | 1:14:A:TRP:HE1 | 2 | 0.52 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 1 | 0.52 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 5 | 0.52 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 5 | 0.52 |
| (1,2773) | 1:10:A:ARG:HG2 | 1:83:A:GLY:H | 2 | 0.52 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 6 | 0.52 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 7 | 0.52 |
| (1,2494) | 1:108:A:GLY:H | 1:111:A:LYS:HE3 | 8 | 0.52 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 4 | 0.52 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 5 | 0.52 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 1 | 0.52 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 8 | 0.52 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 1 | 0.52 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 2 | 0.52 |
| (1,1822) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 6 | 0.52 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 4 | 0.52 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 4 | 0.52 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 4 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 2 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 2 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 2 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 2 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 2 | 0.52 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 2 | 0.52 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 10 | 0.52 |
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 7 | 0.52 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 3 | 0.52 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 3 | 0.52 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 3 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 9 | 0.52 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 9 | 0.52 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 9 | 0.52 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 2 | 0.52 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 2 | 0.52 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 2 | 0.52 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 3 | 0.52 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 3 | 0.52 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 3 | 0.52 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 4 | 0.52 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 4 | 0.52 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 4 | 0.52 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 6 | 0.52 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 10 | 0.52 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 10 | 0.52 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 3 | 0.52 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 1 | 0.52 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 1 | 0.52 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 1 | 0.52 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 3 | 0.52 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 3 | 0.52 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 3 | 0.52 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 4 | 0.52 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 4 | 0.52 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 4 | 0.52 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 7 | 0.52 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 7 | 0.52 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 7 | 0.52 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 10 | 0.52 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 10 | 0.52 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 10 | 0.52 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 8 | 0.52 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 8 | 0.52 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 8 | 0.52 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 1 | 0.52 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 1 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 1 | 0.52 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 4 | 0.52 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 4 | 0.52 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 4 | 0.52 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 4 | 0.52 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 4 | 0.52 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 4 | 0.52 |
| (1,287) | 1:20:A:ILE:HD11 | 1:20:A:ILE:H | 9 | 0.52 |
| (1,287) | 1:20:A:ILE:HD12 | 1:20:A:ILE:H | 9 | 0.52 |
| (1,287) | 1:20:A:ILE:HD13 | 1:20:A:ILE:H | 9 | 0.52 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 7 | 0.52 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 7 | 0.52 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 7 | 0.52 |
| (3,1181) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 3 | 0.51 |
| (3,1157) | 1:80:A:LEU:HD12 | 1:14:A:TRP:HZ3 | 6 | 0.51 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 6 | 0.51 |
| (3,995) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 7 | 0.51 |
| (3,961) | 1:30:A:GLU:HG2 | 1:29:A:GLY:H | 5 | 0.51 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD11 | 7 | 0.51 |
| (3,800) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 1 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 1 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 2 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 3 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 5 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 6 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 7 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 9 | 0.51 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 10 | 0.51 |
| (3,583) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB3 | 2 | 0.51 |
| (3,451) | 1:121:A:GLU:H | 1:118:A:ILE:HG23 | 6 | 0.51 |
| (3,366) | 1:42:A:VAL:HG23 | 1:16:A:GLN:HG2 | 9 | 0.51 |
| (3,300) | 1:11:A:THR:HG22 | 1:13:A:TYR:HE2 | 3 | 0.51 |
| (3,241) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HE22 | 9 | 0.51 |
| (3,240) | 1:109:A:PRO:HA | 1:109:A:PRO:HG2 | 10 | 0.51 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 5 | 0.51 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 1 | 0.51 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 7 | 0.51 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 7 | 0.51 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 8 | 0.51 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 8 | 0.51 |
| (1,3641) | 1:11:A:THR:H | 1:81:A:ASN:HD21 | 3 | 0.51 |
| (1,3508) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 7 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3331) | 1:20:A:ILE:H | 1:124:A:SER:HB3 | 2 | 0.51 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE3 | 3 | 0.51 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 10 | 0.51 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 10 | 0.51 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 10 | 0.51 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 8 | 0.51 |
| (1,2792) | 1:81:A:ASN:H | 1:81:A:ASN:HB3 | 1 | 0.51 |
| (1,2792) | 1:81:A:ASN:H | 1:81:A:ASN:HB3 | 4 | 0.51 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 8 | 0.51 |
| (1,2719) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 1 | 0.51 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 2 | 0.51 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 9 | 0.51 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 9 | 0.51 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 10 | 0.51 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 5 | 0.51 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 7 | 0.51 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 7 | 0.51 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 7 | 0.51 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 8 | 0.51 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 3 | 0.51 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 3 | 0.51 |
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 3 | 0.51 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 2 | 0.51 |
| (1,2162) | 1:115:A:VAL:HG21 | 1:113:A:ARG:HD3 | 1 | 0.51 |
| (1,2162) | 1:115:A:VAL:HG22 | 1:113:A:ARG:HD3 | 1 | 0.51 |
| (1,2162) | 1:115:A:VAL:HG23 | 1:113:A:ARG:HD3 | 1 | 0.51 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 4 | 0.51 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 4 | 0.51 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 4 | 0.51 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 4 | 0.51 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 4 | 0.51 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 4 | 0.51 |
| (1,1520) | 1:91:A:LEU:HD11 | 1:71:A:PRO:HD3 | 3 | 0.51 |
| (1,1520) | 1:91:A:LEU:HD12 | 1:71:A:PRO:HD3 | 3 | 0.51 |
| (1,1520) | 1:91:A:LEU:HD13 | 1:71:A:PRO:HD3 | 3 | 0.51 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 10 | 0.51 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 2 | 0.51 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 6 | 0.51 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 10 | 0.51 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 10 | 0.51 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 10 | 0.51 |
| (1,816) | 1:111:A:LYS:HD3 | 1:106:A:GLU:HA | 7 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 2 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 6 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 7 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 9 | 0.51 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 9 | 0.51 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 7 | 0.51 |
| (1,669) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 8 | 0.51 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 3 | 0.51 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 3 | 0.51 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 3 | 0.51 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 2 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 2 | 0.51 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 2 | 0.51 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 6 | 0.51 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 6 | 0.51 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 6 | 0.51 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 8 | 0.51 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 8 | 0.51 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 8 | 0.51 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 9 | 0.51 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 9 | 0.51 |
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 9 | 0.51 |
| (1,580) | 1:78:A:LEU:HA | 1:78:A:LEU:HD21 | 6 | 0.51 |
| (1,580) | 1:78:A:LEU:HA | 1:78:A:LEU:HD22 | 6 | 0.51 |
| (1,580) | 1:78:A:LEU:HA | 1:78:A:LEU:HD23 | 6 | 0.51 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 2 | 0.51 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 2 | 0.51 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 10 | 0.51 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 10 | 0.51 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 10 | 0.51 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 10 | 0.51 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 10 | 0.51 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 10 | 0.51 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 2 | 0.5 |
| (3,850) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HH2 | 6 | 0.5 |
| (3,849) | 1:26:A:LYS:HB3 | 1:33:A:HIS:H | 2 | 0.5 |
| (3,795) | 1:52:A:MET:H | 1:56:A:GLY:HA3 | 9 | 0.5 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG21 | 5 | 0.5 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 4 | 0.5 |
| (3,673) | 1:73:A:PRO:HA | 1:73:A:PRO:HD2 | 8 | 0.5 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 7 | 0.5 |
| (3,583) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB3 | 7 | 0.5 |
| (3,583) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB3 | 8 | 0.5 |
| (3,568) | 1:78:A:LEU:HD12 | 1:78:A:LEU:HD22 | 7 | 0.5 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 5 | 0.5 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 2 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 4 | 0.5 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 10 | 0.5 |
| (1,3758) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 4 | 0.5 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 9 | 0.5 |
| (1,3725) | 1:95:A:ASN:HD22 | 1:95:A:ASN:H | 2 | 0.5 |
| (1,3648) | 1:16:A:GLN:HE22 | 1:80:A:LEU:HG | 8 | 0.5 |
| (1,3509) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 4 | 0.5 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 5 | 0.5 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 6 | 0.5 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 6 | 0.5 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 3 | 0.5 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 9 | 0.5 |
| (1,2708) | 1:88:A:GLU:HB3 | 1:89:A:GLY:H | 1 | 0.5 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 3 | 0.5 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 2 | 0.5 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 2 | 0.5 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 6 | 0.5 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 6 | 0.5 |
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 6 | 0.5 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 2 | 0.5 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 7 | 0.5 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 7 | 0.5 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 7 | 0.5 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 6 | 0.5 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 6 | 0.5 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 6 | 0.5 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 10 | 0.5 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 10 | 0.5 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 10 | 0.5 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 5 | 0.5 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG21 | 10 | 0.5 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG22 | 10 | 0.5 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG23 | 10 | 0.5 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG21 | 1 | 0.5 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG22 | 1 | 0.5 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG23 | 1 | 0.5 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 9 | 0.5 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 9 | 0.5 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 9 | 0.5 |
| (1,818) | 1:51:A:LYS:HG3 | 1:56:A:GLY:HA3 | 1 | 0.5 |
| (1,636) | 1:42:A:VAL:HG21 | 1:42:A:VAL:HA | 5 | 0.5 |
| (1,636) | 1:42:A:VAL:HG22 | 1:42:A:VAL:HA | 5 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,636) | 1:42:A:VAL:HG23 | 1:42:A:VAL:HA | 5 | 0.5 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 1 | 0.5 |
| (1,458) | 1:61:A:LEU:HD21 | 1:60:A:LYS:H | 7 | 0.5 |
| (1,458) | 1:61:A:LEU:HD22 | 1:60:A:LYS:H | 7 | 0.5 |
| (1,458) | 1:61:A:LEU:HD23 | 1:60:A:LYS:H | 7 | 0.5 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 9 | 0.5 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 9 | 0.5 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 9 | 0.5 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 5 | 0.5 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 5 | 0.5 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 5 | 0.5 |
| (3,1093) | 1:70:A:ILE:HD12 | 1:123:A:ILE:H | 6 | 0.49 |
| (3,919) | 1:65:A:HIS:HE1 | 1:27:A:LYS:HD2 | 8 | 0.49 |
| (3,879) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HB | 2 | 0.49 |
| (3,879) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HB | 3 | 0.49 |
| (3,879) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HB | 4 | 0.49 |
| (3,879) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HB | 8 | 0.49 |
| (3,879) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HB | 9 | 0.49 |
| (3,841) | 1:80:A:LEU:HD22 | 1:80:A:LEU:H | 5 | 0.49 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD11 | 6 | 0.49 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 4 | 0.49 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG23 | 10 | 0.49 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 2 | 0.49 |
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 3 | 0.49 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 9 | 0.49 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 5 | 0.49 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 5 | 0.49 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 2 | 0.49 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 2 | 0.49 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 2 | 0.49 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 1 | 0.49 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 3 | 0.49 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 10 | 0.49 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 10 | 0.49 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 10 | 0.49 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 6 | 0.49 |
| (1,2708) | 1:88:A:GLU:HB3 | 1:89:A:GLY:H | 4 | 0.49 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 2 | 0.49 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 3 | 0.49 |
| (1,2239) | 1:10:A:ARG:HG2 | 1:82:A:GLY:HA3 | 1 | 0.49 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 8 | 0.49 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 8 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 8 | 0.49 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 8 | 0.49 |
| (1,1996) | 1:121:A:GLU:H | 1:121:A:GLU:HB2 | 6 | 0.49 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 5 | 0.49 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 5 | 0.49 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 5 | 0.49 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 5 | 0.49 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 8 | 0.49 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 8 | 0.49 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 8 | 0.49 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 4 | 0.49 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 8 | 0.49 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 8 | 0.49 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 8 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 1 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 1 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 1 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 7 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 7 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 7 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 10 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 10 | 0.49 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 10 | 0.49 |
| (1,893) | 1:51:A:LYS:HG3 | 1:56:A:GLY:HA3 | 1 | 0.49 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 1 | 0.49 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 6 | 0.49 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 6 | 0.49 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 6 | 0.49 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 8 | 0.49 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 8 | 0.49 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 8 | 0.49 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 8 | 0.49 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 1 | 0.49 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 1 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 1 | 0.49 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 2 | 0.49 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 2 | 0.49 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 2 | 0.49 |
| (1,287) | 1:20:A:ILE:HD11 | 1:20:A:ILE:H | 3 | 0.49 |
| (1,287) | 1:20:A:ILE:HD12 | 1:20:A:ILE:H | 3 | 0.49 |
| (1,287) | 1:20:A:ILE:HD13 | 1:20:A:ILE:H | 3 | 0.49 |
| (1,59) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 7 | 0.49 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 7 | 0.48 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HG2 | 4 | 0.48 |
| (3,1098) | 1:55:A:SER:HA | 1:55:A:SER:HB2 | 2 | 0.48 |
| (3,1093) | 1:70:A:ILE:HD11 | 1:123:A:ILE:H | 10 | 0.48 |
| (3,1076) | 1:97:A:LYS:H | 1:97:A:LYS:HD2 | 6 | 0.48 |
| (3,993) | 1:61:A:LEU:HG | 1:50:A:VAL:H | 4 | 0.48 |
| (3,993) | 1:58:A:LYS:HG3 | 1:50:A:VAL:H | 7 | 0.48 |
| (3,879) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HB | 5 | 0.48 |
| (3,879) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HB | 7 | 0.48 |
| (3,879) | 1:49:A:VAL:HB | 1:49:A:VAL:HG23 | 10 | 0.48 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG21 | 2 | 0.48 |
| (3,568) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HD21 | 3 | 0.48 |
| (3,414) | 1:22:A:LYS:HD2 | 1:34:A:LYS:HA | 4 | 0.48 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 4 | 0.48 |
| (3,378) | 1:89:A:GLY:H | 1:105:A:ILE:HD13 | 10 | 0.48 |
| (3,339) | 1:30:A:GLU:HG3 | 1:32:A:TYR:H | 1 | 0.48 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 7 | 0.48 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 5 | 0.48 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 10 | 0.48 |
| (1,3592) | 1:95:A:ASN:HA | 1:95:A:ASN:HD22 | 4 | 0.48 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 2 | 0.48 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 3 | 0.48 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 3 | 0.48 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 3 | 0.48 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 6 | 0.48 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 6 | 0.48 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 6 | 0.48 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 2 | 0.48 |
| (1,3128) | 1:47:A:THR:HB | 1:44:A:ASP:H | 9 | 0.48 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 1 | 0.48 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 6 | 0.48 |
| (1,2721) | 1:75:A:LYS:HB3 | 1:76:A:ARG:H | 10 | 0.48 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 5 | 0.48 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 8 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 6 | 0.48 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 6 | 0.48 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 6 | 0.48 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 7 | 0.48 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 3 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 1 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 1 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 1 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 2 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 2 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 2 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 3 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 3 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 3 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 4 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 4 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 4 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 5 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 5 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 5 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 6 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 6 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 6 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 7 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 7 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 7 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 8 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 8 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 8 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 9 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 9 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 9 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 10 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 10 | 0.48 |
| (1,1347) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 10 | 0.48 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 5 | 0.48 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 9 | 0.48 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 9 | 0.48 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 9 | 0.48 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 3 | 0.48 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 3 | 0.48 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 3 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 9 | 0.48 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 9 | 0.48 |
| (1,1095) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 9 | 0.48 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 2 | 0.48 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 2 | 0.48 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 2 | 0.48 |
| (1,829) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 5 | 0.48 |
| (1,829) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 6 | 0.48 |
| (1,829) | 1:52:A:MET:H | 1:52:A:MET:HG3 | 7 | 0.48 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 7 | 0.48 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 7 | 0.48 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 7 | 0.48 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 1 | 0.48 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 1 | 0.48 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 1 | 0.48 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 6 | 0.48 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 6 | 0.48 |
| (3,1157) | 1:80:A:LEU:HD12 | 1:14:A:TRP:HZ3 | 10 | 0.47 |
| (3,1154) | 1:7:A:ARG:HB2 | 1:7:A:ARG:H | 6 | 0.47 |
| (3,1087) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HB3 | 6 | 0.47 |
| (3,1087) | 1:61:A:LEU:HD12 | 1:59:A:LEU:HB3 | 6 | 0.47 |
| (3,1087) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HB3 | 6 | 0.47 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 3 | 0.47 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 7 | 0.47 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 6 | 0.47 |
| (3,879) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HB | 1 | 0.47 |
| (3,879) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HB | 6 | 0.47 |
| (3,841) | 1:80:A:LEU:HD22 | 1:80:A:LEU:H | 6 | 0.47 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 5 | 0.47 |
| (3,568) | 1:78:A:LEU:HD13 | 1:78:A:LEU:HD22 | 6 | 0.47 |
| (3,568) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HD22 | 8 | 0.47 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 7 | 0.47 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 9 | 0.47 |
| (3,427) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HB2 | 7 | 0.47 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 6 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,611) | 1:123:A:ILE:H | 1:81:A:ASN:HB3 | 3 | 0.47 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 9 | 0.47 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 2 | 0.47 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 2 | 0.47 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 2 | 0.47 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 6 | 0.47 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 5 | 0.47 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 7 | 0.47 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 5 | 0.47 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 5 | 0.47 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 5 | 0.47 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 4 | 0.47 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 9 | 0.47 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 10 | 0.47 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 10 | 0.47 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 10 | 0.47 |
| (1,3245) | 1:30:A:GLU:HG2 | 1:33:A:HIS:H | 4 | 0.47 |
| (1,3015) | 1:32:A:TYR:HE1 | 1:57:A:ASP:H | 8 | 0.47 |
| (1,3015) | 1:32:A:TYR:HE2 | 1:57:A:ASP:H | 8 | 0.47 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 5 | 0.47 |
| (1,2792) | 1:81:A:ASN:H | 1:81:A:ASN:HB3 | 3 | 0.47 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 5 | 0.47 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 10 | 0.47 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 10 | 0.47 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 7 | 0.47 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 9 | 0.47 |
| (1,2571) | 1:117:A:GLY:HA2 | 1:101:A:ALA:H | 4 | 0.47 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 10 | 0.47 |
| (1,2456) | 1:115:A:VAL:HG11 | 1:114:A:ARG:H | 4 | 0.47 |
| (1,2456) | 1:115:A:VAL:HG12 | 1:114:A:ARG:H | 4 | 0.47 |
| (1,2456) | 1:115:A:VAL:HG13 | 1:114:A:ARG:H | 4 | 0.47 |
| (1,2456) | 1:115:A:VAL:HG11 | 1:114:A:ARG:H | 8 | 0.47 |
| (1,2456) | 1:115:A:VAL:HG12 | 1:114:A:ARG:H | 8 | 0.47 |
| (1,2456) | 1:115:A:VAL:HG13 | 1:114:A:ARG:H | 8 | 0.47 |
| (1,2071) | 1:126:A:LEU:HB2 | 1:76:A:ARG:HB3 | 1 | 0.47 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 9 | 0.47 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 9 | 0.47 |
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 9 | 0.47 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 4 | 0.47 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 8 | 0.47 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 8 | 0.47 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 7 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 7 | 0.47 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 7 | 0.47 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 1 | 0.47 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 4 | 0.47 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 6 | 0.47 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 4 | 0.47 |
| (1,1481) | 1:88:A:GLU:HG3 | 1:88:A:GLU:H | 4 | 0.47 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 10 | 0.47 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 10 | 0.47 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 10 | 0.47 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 1 | 0.47 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 9 | 0.47 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 9 | 0.47 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 9 | 0.47 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 9 | 0.47 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 9 | 0.47 |
| (1,1183) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 9 | 0.47 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 7 | 0.47 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG21 | 10 | 0.47 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG22 | 10 | 0.47 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG23 | 10 | 0.47 |
| (1,816) | 1:111:A:LYS:HD3 | 1:106:A:GLU:HA | 1 | 0.47 |
| (1,739) | 1:45:A:LYS:HG2 | 1:45:A:LYS:HE2 | 7 | 0.47 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 8 | 0.47 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 2 | 0.47 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 2 | 0.47 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 2 | 0.47 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 3 | 0.47 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 4 | 0.47 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 4 | 0.47 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 2 | 0.47 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 4 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 4 | 0.47 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 9 | 0.47 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 9 | 0.47 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 2 | 0.47 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 2 | 0.47 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 2 | 0.47 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 8 | 0.47 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 8 | 0.47 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 8 | 0.47 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 1 | 0.47 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 1 | 0.47 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 1 | 0.47 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 8 | 0.47 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 8 | 0.47 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 8 | 0.47 |
| (3,919) | 1:75:A:LYS:HD3 | 1:72:A:ALA:H | 9 | 0.46 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD12 | 9 | 0.46 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 2 | 0.46 |
| (3,568) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HD23 | 1 | 0.46 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 4 | 0.46 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 8 | 0.46 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 9 | 0.46 |
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 1 | 0.46 |
| (3,146) | 1:115:A:VAL:H | 1:114:A:ARG:HG2 | 7 | 0.46 |
| (3,4) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 1 | 0.46 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 2 | 0.46 |
| (1,3835) | 1:62:A:ASP:H | 1:65:A:HIS:HD2 | 8 | 0.46 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 2 | 0.46 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 2 | 0.46 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 2 | 0.46 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 7 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3243) | 1:30:A:GLU:HB2 | 1:33:A:HIS:H | 5 | 0.46 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 6 | 0.46 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 2 | 0.46 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 6 | 0.46 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 7 | 0.46 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 10 | 0.46 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 8 | 0.46 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 3 | 0.46 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 3 | 0.46 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 3 | 0.46 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 3 | 0.46 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 4 | 0.46 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 5 | 0.46 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 7 | 0.46 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 10 | 0.46 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 3 | 0.46 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 5 | 0.46 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 9 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 7 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 7 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 7 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 7 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 7 | 0.46 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 7 | 0.46 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 6 | 0.46 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 5 | 0.46 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 5 | 0.46 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 5 | 0.46 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 7 | 0.46 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 8 | 0.46 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 10 | 0.46 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 5 | 0.46 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 6 | 0.46 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 6 | 0.46 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 6 | 0.46 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 10 | 0.46 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 10 | 0.46 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 10 | 0.46 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 8 | 0.46 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 4 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 1 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 1 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 1 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 3 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 3 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 3 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 5 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 5 | 0.46 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 5 | 0.46 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 2 | 0.46 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 2 | 0.46 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 2 | 0.46 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 8 | 0.46 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 8 | 0.46 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 8 | 0.46 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG21 | 2 | 0.46 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG22 | 2 | 0.46 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG23 | 2 | 0.46 |
| (3,1155) | 1:118:A:ILE:HG21 | 1:119:A:GLN:H | 7 | 0.45 |
| (3,1113) | 1:81:A:ASN:HD22 | 1:14:A:TRP:HB3 | 5 | 0.45 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 7 | 0.45 |
| (3,951) | 1:80:A:LEU:HD12 | 1:124:A:SER:H | 5 | 0.45 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 5 | 0.45 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG21 | 8 | 0.45 |
| (3,568) | 1:19:A:ILE:HG22 | 1:78:A:LEU:HD12 | 5 | 0.45 |
| (3,568) | 1:19:A:ILE:HG23 | 1:78:A:LEU:HD12 | 10 | 0.45 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 3 | 0.45 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 1 | 0.45 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 3 | 0.45 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 9 | 0.45 |
| (3,22) | 1:9:A:ALA:HB1 | 1:11:A:THR:H | 2 | 0.45 |
| (2,574) | 1:39:A:VAL:H | 1:20:A:ILE:HG12 | 10 | 0.45 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 3 | 0.45 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 3 | 0.45 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 3 | 0.45 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG11 | 8 | 0.45 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG12 | 8 | 0.45 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG13 | 8 | 0.45 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 10 | 0.45 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 10 | 0.45 |
| (1,3737) | 1:5:A:LYS:H | 1:3:A:GLU:H | 3 | 0.45 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 9 | 0.45 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 3 | 0.45 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 5 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 3 | 0.45 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 3 | 0.45 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 3 | 0.45 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 7 | 0.45 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 7 | 0.45 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 7 | 0.45 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 7 | 0.45 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 10 | 0.45 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 6 | 0.45 |
| (1,3027) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 2 | 0.45 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 4 | 0.45 |
| (1,2887) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 4 | 0.45 |
| (1,2859) | 1:75:A:LYS:HE2 | 1:75:A:LYS:H | 5 | 0.45 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 2 | 0.45 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 5 | 0.45 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 5 | 0.45 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 5 | 0.45 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 2 | 0.45 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 4 | 0.45 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 8 | 0.45 |
| (1,2461) | 1:84:A:TYR:HE1 | 1:113:A:ARG:H | 2 | 0.45 |
| (1,2461) | 1:84:A:TYR:HE2 | 1:113:A:ARG:H | 2 | 0.45 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 2 | 0.45 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 1 | 0.45 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 1 | 0.45 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 1 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 10 | 0.45 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 10 | 0.45 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 8 | 0.45 |
| (1,2162) | 1:115:A:VAL:HG21 | 1:113:A:ARG:HD3 | 5 | 0.45 |
| (1,2162) | 1:115:A:VAL:HG22 | 1:113:A:ARG:HD3 | 5 | 0.45 |
| (1,2162) | 1:115:A:VAL:HG23 | 1:113:A:ARG:HD3 | 5 | 0.45 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 1 | 0.45 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 1 | 0.45 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 1 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 6 | 0.45 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 6 | 0.45 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 6 | 0.45 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 10 | 0.45 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 10 | 0.45 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 10 | 0.45 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 6 | 0.45 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 9 | 0.45 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 6 | 0.45 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 7 | 0.45 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 8 | 0.45 |
| (1,1603) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 10 | 0.45 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 9 | 0.45 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 3 | 0.45 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 9 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 1 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 1 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 1 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 2 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 2 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 2 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 3 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 3 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 3 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 4 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 4 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 4 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 5 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 5 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 5 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 7 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 7 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 7 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 8 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 8 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 8 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG21 | 9 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG22 | 9 | 0.45 |
| (1,1184) | 1:70:A:ILE:HG12 | 1:70:A:ILE:HG23 | 9 | 0.45 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 1 | 0.45 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 2 | 0.45 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 2 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 2 | 0.45 |
| (1,739) | 1:45:A:LYS:HG2 | 1:45:A:LYS:HE2 | 5 | 0.45 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 7 | 0.45 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 8 | 0.45 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 8 | 0.45 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 8 | 0.45 |
| (1,290) | 1:20:A:ILE:HG13 | 1:127:A:ALA:HA | 5 | 0.45 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 3 | 0.45 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 3 | 0.45 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 3 | 0.45 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 3 | 0.45 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 3 | 0.45 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 3 | 0.45 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 6 | 0.45 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 6 | 0.45 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 6 | 0.45 |
| (1,82) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 10 | 0.45 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 1 | 0.44 |
| (3,1184) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 2 | 0.44 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 2 | 0.44 |
| (3,1087) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HB3 | 5 | 0.44 |
| (3,1087) | 1:61:A:LEU:HD12 | 1:59:A:LEU:HB3 | 5 | 0.44 |
| (3,1087) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HB3 | 5 | 0.44 |
| (3,995) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 10 | 0.44 |
| (3,951) | 1:80:A:LEU:HD11 | 1:124:A:SER:H | 10 | 0.44 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 3 | 0.44 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 4 | 0.44 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 9 | 0.44 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 6 | 0.44 |
| (3,582) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 3 | 0.44 |
| (3,561) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HB2 | 8 | 0.44 |
| (3,518) | 1:26:A:LYS:HD2 | 1:30:A:GLU:HG2 | 1 | 0.44 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 1 | 0.44 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 6 | 0.44 |
| (3,300) | 1:11:A:THR:HG23 | 1:13:A:TYR:HE2 | 2 | 0.44 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 6 | 0.44 |
| (3,165) | 1:79:A:VAL:HG12 | 1:88:A:GLU:HA | 6 | 0.44 |
| (3,153) | 1:91:A:LEU:HD11 | 1:102:A:THR:H | 4 | 0.44 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 3 | 0.44 |
| (1,3777) | 1:45:A:LYS:HG2 | 1:46:A:TYR:HD1 | 4 | 0.44 |
| (1,3777) | 1:45:A:LYS:HG2 | 1:46:A:TYR:HD2 | 4 | 0.44 |
| (1,3714) | 1:84:A:TYR:HD1 | 1:87:A:ASN:HD22 | 5 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3714) | 1:84:A:TYR:HD2 | 1:87:A:ASN:HD22 | 5 | 0.44 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 1 | 0.44 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 3 | 0.44 |
| (1,3599) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD22 | 7 | 0.44 |
| (1,3599) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD22 | 7 | 0.44 |
| (1,3599) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD22 | 7 | 0.44 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 3 | 0.44 |
| (1,3460) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HE22 | 8 | 0.44 |
| (1,3460) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HE22 | 8 | 0.44 |
| (1,3460) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HE22 | 8 | 0.44 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 9 | 0.44 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 9 | 0.44 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 9 | 0.44 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 2 | 0.44 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD11 | 10 | 0.44 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD12 | 10 | 0.44 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD13 | 10 | 0.44 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 1 | 0.44 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 2 | 0.44 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 4 | 0.44 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 7 | 0.44 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 3 | 0.44 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 8 | 0.44 |
| (1,2621) | 1:97:A:LYS:H | 1:97:A:LYS:HD3 | 2 | 0.44 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 5 | 0.44 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 2 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 2 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 2 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 2 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 4 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 4 | 0.44 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 4 | 0.44 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 7 | 0.44 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 7 | 0.44 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 7 | 0.44 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 7 | 0.44 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 7 | 0.44 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 7 | 0.44 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 6 | 0.44 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 6 | 0.44 |
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 6 | 0.44 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 10 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 6 | 0.44 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 6 | 0.44 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 6 | 0.44 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 1 | 0.44 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 1 | 0.44 |
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 1 | 0.44 |
| (1,1892) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 10 | 0.44 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 1 | 0.44 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 1 | 0.44 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 1 | 0.44 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 8 | 0.44 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 1 | 0.44 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 3 | 0.44 |
| (1,1492) | 1:104:A:VAL:H | 1:90:A:THR:HB | 3 | 0.44 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 1 | 0.44 |
| (1,1275) | 1:97:A:LYS:H | 1:97:A:LYS:HB3 | 4 | 0.44 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 8 | 0.44 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 8 | 0.44 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 8 | 0.44 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG21 | 7 | 0.44 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG22 | 7 | 0.44 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG23 | 7 | 0.44 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 10 | 0.44 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 10 | 0.44 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 2 | 0.44 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 4 | 0.44 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 5 | 0.44 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 6 | 0.44 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 9 | 0.44 |
| (1,621) | 1:41:A:GLU:HA | 1:41:A:GLU:HG3 | 6 | 0.44 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 7 | 0.44 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 8 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 8 | 0.44 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 8 | 0.44 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 7 | 0.44 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 7 | 0.44 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 7 | 0.44 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 1 | 0.44 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 1 | 0.44 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 1 | 0.44 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 9 | 0.44 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 9 | 0.44 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 9 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 2 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 8 | 0.44 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 8 | 0.44 |
| (1,287) | 1:20:A:ILE:HD11 | 1:20:A:ILE:H | 4 | 0.44 |
| (1,287) | 1:20:A:ILE:HD12 | 1:20:A:ILE:H | 4 | 0.44 |
| (1,287) | 1:20:A:ILE:HD13 | 1:20:A:ILE:H | 4 | 0.44 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 8 | 0.44 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 8 | 0.44 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 8 | 0.44 |
| (1,170) | 1:78:A:LEU:HD11 | 1:16:A:GLN:HG3 | 2 | 0.44 |
| (1,170) | 1:78:A:LEU:HD12 | 1:16:A:GLN:HG3 | 2 | 0.44 |
| (1,170) | 1:78:A:LEU:HD13 | 1:16:A:GLN:HG3 | 2 | 0.44 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 2 | 0.44 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 2 | 0.44 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 3 | 0.43 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 6 | 0.43 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 5 | 0.43 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 10 | 0.43 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD13 | 3 | 0.43 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD11 | 4 | 0.43 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD11 | 6 | 0.43 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD13 | 9 | 0.43 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG22 | 10 | 0.43 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 10 | 0.43 |
| (3,751) | 1:43:A:ILE:HG23 | 1:43:A:ILE:H | 7 | 0.43 |
| (3,680) | 1:64:A:THR:H | 1:24:A:ILE:HD11 | 10 | 0.43 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 2 | 0.43 |
| (3,568) | 1:19:A:ILE:HG22 | 1:78:A:LEU:HD12 | 9 | 0.43 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 7 | 0.43 |
| (3,471) | 1:127:A:ALA:HB2 | 1:20:A:ILE:H | 10 | 0.43 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 6 | 0.43 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 5 | 0.43 |
| (3,174) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 8 | 0.43 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 10 | 0.43 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 10 | 0.43 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 10 | 0.43 |
| (2,351) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HB3 | 2 | 0.43 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 1 | 0.43 |
| (1,3842) | 1:46:A:TYR:HE1 | 1:45:A:LYS:HB2 | 4 | 0.43 |
| (1,3842) | 1:46:A:TYR:HE2 | 1:45:A:LYS:HB2 | 4 | 0.43 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 10 | 0.43 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 10 | 0.43 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 6 | 0.43 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 6 | 0.43 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 6 | 0.43 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 8 | 0.43 |
| (1,3599) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD22 | 3 | 0.43 |
| (1,3599) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD22 | 3 | 0.43 |
| (1,3599) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD22 | 3 | 0.43 |
| (1,3557) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HD21 | 5 | 0.43 |
| (1,3417) | 1:7:A:ARG:HD3 | 1:8:A:THR:H | 2 | 0.43 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 1 | 0.43 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 4 | 0.43 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 4 | 0.43 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 10 | 0.43 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 10 | 0.43 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 10 | 0.43 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD11 | 2 | 0.43 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD12 | 2 | 0.43 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD13 | 2 | 0.43 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 6 | 0.43 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 10 | 0.43 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 4 | 0.43 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 10 | 0.43 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 8 | 0.43 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 4 | 0.43 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 3 | 0.43 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 3 | 0.43 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 6 | 0.43 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 2 | 0.43 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 1 | 0.43 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 1 | 0.43 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 3 | 0.43 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 9 | 0.43 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 9 | 0.43 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 4 | 0.43 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 4 | 0.43 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 4 | 0.43 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 2 | 0.43 |
| (1,1963) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HB | 6 | 0.43 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 9 | 0.43 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 3 | 0.43 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 2 | 0.43 |
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 10 | 0.43 |
| (1,816) | 1:111:A:LYS:HD3 | 1:106:A:GLU:HA | 4 | 0.43 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 8 | 0.43 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 8 | 0.43 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 9 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 1 | 0.43 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 10 | 0.43 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 5 | 0.43 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 5 | 0.43 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 4 | 0.43 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 4 | 0.43 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 4 | 0.43 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 10 | 0.43 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 10 | 0.43 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 10 | 0.43 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 10 | 0.43 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 10 | 0.43 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 10 | 0.43 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 8 | 0.43 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 8 | 0.43 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 9 | 0.43 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 9 | 0.43 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 9 | 0.43 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 8 | 0.43 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 8 | 0.43 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 8 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 2 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 2 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 2 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 3 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 3 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 3 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 4 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 4 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 5 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 5 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 5 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 6 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 6 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 6 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 7 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 7 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 7 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 8 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 8 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 8 | 0.43 |
| (1,367) | 1:23:A:ILE:HG21 | 1:23:A:ILE:HG13 | 10 | 0.43 |
| (1,367) | 1:23:A:ILE:HG22 | 1:23:A:ILE:HG13 | 10 | 0.43 |
| (1,367) | 1:23:A:ILE:HG23 | 1:23:A:ILE:HG13 | 10 | 0.43 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 4 | 0.43 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 4 | 0.43 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 4 | 0.43 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 5 | 0.43 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 5 | 0.43 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 5 | 0.43 |
| (3,1221) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HD11 | 3 | 0.42 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 8 | 0.42 |
| (3,1172) | 1:118:A:ILE:HG12 | 1:103:A:ILE:HG13 | 3 | 0.42 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 10 | 0.42 |
| (3,1093) | 1:70:A:ILE:HD13 | 1:123:A:ILE:H | 1 | 0.42 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 4 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD13 | 2 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD13 | 5 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD13 | 7 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD12 | 8 | 0.42 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD12 | 10 | 0.42 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 2 | 0.42 |
| (3,751) | 1:43:A:ILE:HG22 | 1:43:A:ILE:H | 1 | 0.42 |
| (3,751) | 1:43:A:ILE:HG21 | 1:43:A:ILE:H | 10 | 0.42 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 5 | 0.42 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 8 | 0.42 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 2 | 0.42 |
| (3,401) | 1:15:A:LEU:HD22 | 1:80:A:LEU:HD13 | 2 | 0.42 |
| (3,371) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 2 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 5 | 0.42 |
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 8 | 0.42 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD13 | 8 | 0.42 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 2 | 0.42 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 2 | 0.42 |
| (1,3522) | 1:40:A:LYS:HE3 | 1:51:A:LYS:H | 4 | 0.42 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 4 | 0.42 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 10 | 0.42 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 7 | 0.42 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 8 | 0.42 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 7 | 0.42 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 4 | 0.42 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 1 | 0.42 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 2 | 0.42 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 5 | 0.42 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 4 | 0.42 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 1 | 0.42 |
| (1,2323) | 1:126:A:LEU:H | 1:71:A:PRO:HD2 | 1 | 0.42 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 9 | 0.42 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 3 | 0.42 |
| (1,2232) | 1:78:A:LEU:HD11 | 1:78:A:LEU:HB3 | 6 | 0.42 |
| (1,2232) | 1:78:A:LEU:HD12 | 1:78:A:LEU:HB3 | 6 | 0.42 |
| (1,2232) | 1:78:A:LEU:HD13 | 1:78:A:LEU:HB3 | 6 | 0.42 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 1 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 5 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 5 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 5 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 5 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 5 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 5 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 8 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 8 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 8 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 8 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 8 | 0.42 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 8 | 0.42 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 2 | 0.42 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 8 | 0.42 |
| (1,1527) | 1:93:A:SER:H | 1:91:A:LEU:HG | 1 | 0.42 |
| (1,1484) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 10 | 0.42 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 7 | 0.42 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 5 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 9 | 0.42 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 8 | 0.42 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 8 | 0.42 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 8 | 0.42 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 3 | 0.42 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 3 | 0.42 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 5 | 0.42 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 5 | 0.42 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 5 | 0.42 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 5 | 0.42 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 5 | 0.42 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 5 | 0.42 |
| (1,739) | 1:45:A:LYS:HG2 | 1:45:A:LYS:HE2 | 3 | 0.42 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG21 | 7 | 0.42 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG22 | 7 | 0.42 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG23 | 7 | 0.42 |
| (1,703) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 7 | 0.42 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 10 | 0.42 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 10 | 0.42 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 10 | 0.42 |
| (1,693) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 9 | 0.42 |
| (1,693) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 9 | 0.42 |
| (1,693) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 9 | 0.42 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 3 | 0.42 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 3 | 0.42 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 3 | 0.42 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 10 | 0.42 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 10 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG11 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG12 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD21 | 1:39:A:VAL:HG13 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG11 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG12 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD22 | 1:39:A:VAL:HG13 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG11 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG12 | 1 | 0.42 |
| (1,577) | 1:15:A:LEU:HD23 | 1:39:A:VAL:HG13 | 1 | 0.42 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 9 | 0.42 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 9 | 0.42 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 9 | 0.42 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 9 | 0.42 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 5 | 0.42 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 5 | 0.42 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 5 | 0.42 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 8 | 0.42 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 8 | 0.42 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 8 | 0.42 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 7 | 0.42 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 7 | 0.42 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 7 | 0.42 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 1 | 0.42 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 1 | 0.42 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 1 | 0.42 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 3 | 0.42 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 3 | 0.42 |
| (1,290) | 1:20:A:ILE:HG13 | 1:127:A:ALA:HA | 6 | 0.42 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 5 | 0.42 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 5 | 0.42 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 5 | 0.42 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 3 | 0.42 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 3 | 0.42 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 3 | 0.42 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 1 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 1 | 0.42 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 1 | 0.42 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 4 | 0.42 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 4 | 0.42 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 4 | 0.42 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 4 | 0.41 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 9 | 0.41 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 9 | 0.41 |
| (3,1093) | 1:70:A:ILE:HD12 | 1:123:A:ILE:H | 3 | 0.41 |
| (3,1093) | 1:70:A:ILE:HD13 | 1:123:A:ILE:H | 8 | 0.41 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 10 | 0.41 |
| (3,981) | 1:38:A:ILE:HG13 | 1:38:A:ILE:HD12 | 1 | 0.41 |
| (3,961) | 1:30:A:GLU:HG2 | 1:29:A:GLY:H | 9 | 0.41 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG21 | 6 | 0.41 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 8 | 0.41 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG22 | 1 | 0.41 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 1 | 0.41 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 9 | 0.41 |
| (3,371) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 10 | 0.41 |
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 9 | 0.41 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 1 | 0.41 |
| (3,162) | 1:15:A:LEU:H | 1:19:A:ILE:HD13 | 8 | 0.41 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 5 | 0.41 |
| (2,590) | 1:7:A:ARG:HB2 | 1:9:A:ALA:H | 4 | 0.41 |
| (2,566) | 1:63:A:GLN:HB2 | 1:46:A:TYR:H | 8 | 0.41 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 10 | 0.41 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG11 | 9 | 0.41 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG12 | 9 | 0.41 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG13 | 9 | 0.41 |
| (1,3782) | 1:11:A:THR:HB | 1:13:A:TYR:HD1 | 4 | 0.41 |
| (1,3782) | 1:11:A:THR:HB | 1:13:A:TYR:HD2 | 4 | 0.41 |
| (1,3725) | 1:95:A:ASN:HD22 | 1:95:A:ASN:H | 4 | 0.41 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 7 | 0.41 |
| (1,3695) | 1:68:A:THR:H | 1:121:A:GLU:HB3 | 1 | 0.41 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 4 | 0.41 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 4 | 0.41 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 4 | 0.41 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 7 | 0.41 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 7 | 0.41 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 7 | 0.41 |
| (1,3434) | 1:63:A:GLN:HE22 | 1:14:A:TRP:HE1 | 8 | 0.41 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 9 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 3 | 0.41 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 2 | 0.41 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 7 | 0.41 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 3 | 0.41 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 5 | 0.41 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 6 | 0.41 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 8 | 0.41 |
| (1,2456) | 1:115:A:VAL:HG11 | 1:114:A:ARG:H | 6 | 0.41 |
| (1,2456) | 1:115:A:VAL:HG12 | 1:114:A:ARG:H | 6 | 0.41 |
| (1,2456) | 1:115:A:VAL:HG13 | 1:114:A:ARG:H | 6 | 0.41 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 6 | 0.41 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 5 | 0.41 |
| (1,2292) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB3 | 2 | 0.41 |
| (1,2292) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB3 | 2 | 0.41 |
| (1,2292) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB3 | 2 | 0.41 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 4 | 0.41 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 7 | 0.41 |
| (1,2162) | 1:115:A:VAL:HG21 | 1:113:A:ARG:HD3 | 2 | 0.41 |
| (1,2162) | 1:115:A:VAL:HG22 | 1:113:A:ARG:HD3 | 2 | 0.41 |
| (1,2162) | 1:115:A:VAL:HG23 | 1:113:A:ARG:HD3 | 2 | 0.41 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 4 | 0.41 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 7 | 0.41 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 8 | 0.41 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 8 | 0.41 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 8 | 0.41 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 9 | 0.41 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 9 | 0.41 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 9 | 0.41 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 4 | 0.41 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 4 | 0.41 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 4 | 0.41 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 9 | 0.41 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 9 | 0.41 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 9 | 0.41 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 5 | 0.41 |
| (1,1484) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 4 | 0.41 |
| (1,1484) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 5 | 0.41 |
| (1,1484) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 8 | 0.41 |
| (1,1484) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HA | 9 | 0.41 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 9 | 0.41 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 4 | 0.41 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 1 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 7 | 0.41 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 10 | 0.41 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 6 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 1 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 2 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 5 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 6 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 8 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 9 | 0.41 |
| (1,708) | 1:44:A:ASP:HB3 | 1:44:A:ASP:HA | 10 | 0.41 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 1 | 0.41 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 1 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 5 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 7 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 7 | 0.41 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 7 | 0.41 |
| (1,290) | 1:20:A:ILE:HG13 | 1:127:A:ALA:HA | 10 | 0.41 |
| (1,287) | 1:20:A:ILE:HD11 | 1:20:A:ILE:H | 2 | 0.41 |
| (1,287) | 1:20:A:ILE:HD12 | 1:20:A:ILE:H | 2 | 0.41 |
| (1,287) | 1:20:A:ILE:HD13 | 1:20:A:ILE:H | 2 | 0.41 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 4 | 0.41 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 4 | 0.41 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 4 | 0.41 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 10 | 0.41 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 10 | 0.41 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 10 | 0.41 |
| (1,18) | 1:97:A:LYS:HG3 | 1:97:A:LYS:HA | 5 | 0.41 |
| (1,18) | 1:97:A:LYS:HG3 | 1:97:A:LYS:HA | 8 | 0.41 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 2 | 0.4 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 5 | 0.4 |
| (3,1189) | 1:78:A:LEU:HA | 1:79:A:VAL:HB | 10 | 0.4 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 6 | 0.4 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 4 | 0.4 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 8 | 0.4 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 7 | 0.4 |
| (3,1093) | 1:70:A:ILE:HD11 | 1:123:A:ILE:H | 4 | 0.4 |
| (3,1060) | 1:9:A:ALA:HB3 | 1:9:A:ALA:H | 4 | 0.4 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 1 | 0.4 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 7 | 0.4 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 4 | 0.4 |
| (3,849) | 1:35:A:LYS:HD2 | 1:33:A:HIS:H | 3 | 0.4 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG23 | 3 | 0.4 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG23 | 6 | 0.4 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 6 | 0.4 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 8 | 0.4 |
| (3,345) | 1:35:A:LYS:H | 1:22:A:LYS:HG3 | 6 | 0.4 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 8 | 0.4 |
| (3,280) | 1:112:A:GLY:H | 1:111:A:LYS:HG3 | 4 | 0.4 |
| (3,174) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 9 | 0.4 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 3 | 0.4 |
| (1,3725) | 1:95:A:ASN:HD22 | 1:95:A:ASN:H | 1 | 0.4 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 2 | 0.4 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 5 | 0.4 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 2 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 2 | 0.4 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 2 | 0.4 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 9 | 0.4 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 9 | 0.4 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 9 | 0.4 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 4 | 0.4 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 4 | 0.4 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 4 | 0.4 |
| (1,3434) | 1:63:A:GLN:HE22 | 1:14:A:TRP:HE1 | 5 | 0.4 |
| (1,3403) | 1:10:A:ARG:HD2 | 1:10:A:ARG:H | 6 | 0.4 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 1 | 0.4 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 1 | 0.4 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 1 | 0.4 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE2 | 1 | 0.4 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE2 | 10 | 0.4 |
| (1,3098) | 1:44:A:ASP:HB2 | 1:47:A:THR:H | 2 | 0.4 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 2 | 0.4 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 7 | 0.4 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 9 | 0.4 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 4 | 0.4 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 5 | 0.4 |
| (1,2646) | 1:95:A:ASN:HB3 | 1:95:A:ASN:H | 10 | 0.4 |
| (1,2636) | 1:96:A:GLU:H | 1:97:A:LYS:HD2 | 7 | 0.4 |
| (1,2456) | 1:115:A:VAL:HG11 | 1:114:A:ARG:H | 9 | 0.4 |
| (1,2456) | 1:115:A:VAL:HG12 | 1:114:A:ARG:H | 9 | 0.4 |
| (1,2456) | 1:115:A:VAL:HG13 | 1:114:A:ARG:H | 9 | 0.4 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 5 | 0.4 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 10 | 0.4 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD2 | 10 | 0.4 |
| (1,2162) | 1:115:A:VAL:HG21 | 1:113:A:ARG:HD3 | 3 | 0.4 |
| (1,2162) | 1:115:A:VAL:HG22 | 1:113:A:ARG:HD3 | 3 | 0.4 |
| (1,2162) | 1:115:A:VAL:HG23 | 1:113:A:ARG:HD3 | 3 | 0.4 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 10 | 0.4 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 10 | 0.4 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 10 | 0.4 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 1 | 0.4 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 1 | 0.4 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 1 | 0.4 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 10 | 0.4 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 3 | 0.4 |
| (1,1896) | 1:114:A:ARG:HA | 1:114:A:ARG:HG2 | 7 | 0.4 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 10 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 10 | 0.4 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 10 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB1 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB2 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB3 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB1 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB2 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB3 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB1 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB2 | 1 | 0.4 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 1 | 0.4 |
| (1,1484) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 3 | 0.4 |
| (1,1484) | 1:96:A:GLU:HG2 | 1:96:A:GLU:HA | 7 | 0.4 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 1 | 0.4 |
| (1,1258) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 3 | 0.4 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 2 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 2 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 3 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 4 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 5 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 6 | 0.4 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 8 | 0.4 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 7 | 0.4 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 4 | 0.4 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 4 | 0.4 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 4 | 0.4 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 4 | 0.4 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 4 | 0.4 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 4 | 0.4 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 6 | 0.4 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 6 | 0.4 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 6 | 0.4 |
| (1,816) | 1:111:A:LYS:HD3 | 1:106:A:GLU:HA | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG11 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG12 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HG13 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG11 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG12 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HG13 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG11 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG12 | 10 | 0.4 |
| (1,314) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HG13 | 10 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,290) | 1:20:A:ILE:HG13 | 1:127:A:ALA:HA | 1 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 1 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 1 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 1 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 2 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 2 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 2 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 3 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 3 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 3 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 4 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 4 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 4 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 5 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 5 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 5 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 7 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 7 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 7 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 8 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 8 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 8 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 9 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 9 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 9 | 0.4 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 10 | 0.4 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 10 | 0.4 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 10 | 0.4 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 1 | 0.4 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 1 | 0.4 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 1 | 0.4 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 10 | 0.4 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 10 | 0.4 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 10 | 0.4 |
| (3,1183) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 3 | 0.39 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 1 | 0.39 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 3 | 0.39 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 7 | 0.39 |
| (3,1087) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HB3 | 2 | 0.39 |
| (3,1087) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HB3 | 2 | 0.39 |
| (3,1087) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HB3 | 2 | 0.39 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 9 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG22 | 9 | 0.39 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG22 | 10 | 0.39 |
| (3,628) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 3 | 0.39 |
| (3,628) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 5 | 0.39 |
| (3,537) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 6 | 0.39 |
| (3,440) | 1:103:A:ILE:H | 1:117:A:GLY:H | 4 | 0.39 |
| (3,371) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 3 | 0.39 |
| (3,366) | 1:42:A:VAL:HG23 | 1:16:A:GLN:HG2 | 8 | 0.39 |
| (3,165) | 1:79:A:VAL:HG11 | 1:88:A:GLU:HA | 3 | 0.39 |
| (3,129) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HB | 10 | 0.39 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 4 | 0.39 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 4 | 0.39 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 9 | 0.39 |
| (1,3648) | 1:16:A:GLN:HE22 | 1:80:A:LEU:HG | 3 | 0.39 |
| (1,3648) | 1:16:A:GLN:HE22 | 1:80:A:LEU:HG | 7 | 0.39 |
| (1,3590) | 1:97:A:LYS:HB3 | 1:95:A:ASN:HD21 | 4 | 0.39 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 1 | 0.39 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 7 | 0.39 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 7 | 0.39 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 7 | 0.39 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 4 | 0.39 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 4 | 0.39 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 4 | 0.39 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 5 | 0.39 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 5 | 0.39 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 5 | 0.39 |
| (1,3163) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 5 | 0.39 |
| (1,3163) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 5 | 0.39 |
| (1,3163) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 5 | 0.39 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 2 | 0.39 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 2 | 0.39 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 2 | 0.39 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 5 | 0.39 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 6 | 0.39 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 3 | 0.39 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 10 | 0.39 |
| (1,2878) | 1:75:A:LYS:HE3 | 1:72:A:ALA:H | 9 | 0.39 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 10 | 0.39 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 1 | 0.39 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 1 | 0.39 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 1 | 0.39 |
| (1,2604) | 1:95:A:ASN:HB2 | 1:99:A:PHE:H | 1 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2517) | 1:88:A:GLU:HB2 | 1:106:A:GLU:H | 4 | 0.39 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 10 | 0.39 |
| (1,2456) | 1:115:A:VAL:HG11 | 1:114:A:ARG:H | 10 | 0.39 |
| (1,2456) | 1:115:A:VAL:HG12 | 1:114:A:ARG:H | 10 | 0.39 |
| (1,2456) | 1:115:A:VAL:HG13 | 1:114:A:ARG:H | 10 | 0.39 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 7 | 0.39 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 7 | 0.39 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 6 | 0.39 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 6 | 0.39 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 6 | 0.39 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 6 | 0.39 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 2 | 0.39 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 6 | 0.39 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 8 | 0.39 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 8 | 0.39 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 8 | 0.39 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 9 | 0.39 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 4 | 0.39 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 4 | 0.39 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 4 | 0.39 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 4 | 0.39 |
| (1,1810) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD2 | 10 | 0.39 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 1 | 0.39 |
| (1,1539) | 1:92:A:GLU:HA | 1:92:A:GLU:HG3 | 10 | 0.39 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 2 | 0.39 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 1 | 0.39 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 1 | 0.39 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 1 | 0.39 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 7 | 0.39 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 7 | 0.39 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 7 | 0.39 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 10 | 0.39 |
| (1,1037) | 1:63:A:GLN:HG2 | 1:64:A:THR:HA | 8 | 0.39 |
| (1,1019) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 9 | 0.39 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 5 | 0.39 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 5 | 0.39 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 5 | 0.39 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 2 | 0.39 |
| (1,834) | 1:52:A:MET:HG2 | 1:59:A:LEU:HG | 3 | 0.39 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 3 | 0.39 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 3 | 0.39 |
| (1,633) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 3 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 10 | 0.39 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 10 | 0.39 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 10 | 0.39 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 8 | 0.39 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 8 | 0.39 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 8 | 0.39 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 1 | 0.39 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 2 | 0.39 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 7 | 0.39 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 4 | 0.39 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 4 | 0.39 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 4 | 0.39 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 2 | 0.39 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 2 | 0.39 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 3 | 0.39 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 3 | 0.39 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 3 | 0.39 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 2 | 0.39 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 2 | 0.39 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 2 | 0.39 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 5 | 0.39 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 5 | 0.39 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 5 | 0.39 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 7 | 0.39 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 7 | 0.39 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 7 | 0.39 |
| (1,147) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HB2 | 6 | 0.39 |
| (1,147) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HB2 | 6 | 0.39 |
| (1,147) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HB2 | 6 | 0.39 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 2 | 0.39 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 4 | 0.38 |
| (3,1157) | 1:80:A:LEU:HD11 | 1:14:A:TRP:HZ3 | 8 | 0.38 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG21 | 4 | 0.38 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 5 | 0.38 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG23 | 8 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 9 | 0.38 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD11 | 1 | 0.38 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD12 | 1 | 0.38 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD13 | 1 | 0.38 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 8 | 0.38 |
| (3,751) | 1:43:A:ILE:HG22 | 1:43:A:ILE:H | 4 | 0.38 |
| (3,732) | 1:48:A:ALA:HB3 | 1:43:A:ILE:H | 3 | 0.38 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG23 | 7 | 0.38 |
| (3,628) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 7 | 0.38 |
| (3,628) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 8 | 0.38 |
| (3,628) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 10 | 0.38 |
| (3,600) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 2 | 0.38 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 9 | 0.38 |
| (3,600) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 10 | 0.38 |
| (3,564) | 1:34:A:LYS:HE2 | 1:34:A:LYS:HG2 | 3 | 0.38 |
| (3,537) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 5 | 0.38 |
| (3,471) | 1:127:A:ALA:HB1 | 1:20:A:ILE:H | 4 | 0.38 |
| (3,471) | 1:24:A:ILE:H | 1:24:A:ILE:HG13 | 5 | 0.38 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 10 | 0.38 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 4 | 0.38 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 2 | 0.38 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 8 | 0.38 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 9 | 0.38 |
| (2,520) | 1:78:A:LEU:H | 1:88:A:GLU:HG2 | 4 | 0.38 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 1 | 0.38 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 1 | 0.38 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 1 | 0.38 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 8 | 0.38 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 8 | 0.38 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 8 | 0.38 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 3 | 0.38 |
| (2,142) | 1:10:A:ARG:HA | 1:82:A:GLY:HA3 | 7 | 0.38 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 8 | 0.38 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 1 | 0.38 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 9 | 0.38 |
| (1,3695) | 1:68:A:THR:H | 1:121:A:GLU:HB2 | 10 | 0.38 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 6 | 0.38 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 9 | 0.38 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 8 | 0.38 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 8 | 0.38 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 8 | 0.38 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 3 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 3 | 0.38 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 3 | 0.38 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 9 | 0.38 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 2 | 0.38 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 2 | 0.38 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 2 | 0.38 |
| (1,2841) | 1:111:A:LYS:HE2 | 1:112:A:GLY:H | 4 | 0.38 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 4 | 0.38 |
| (1,2784) | 1:82:A:GLY:H | 1:10:A:ARG:HG2 | 4 | 0.38 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 4 | 0.38 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 6 | 0.38 |
| (1,2572) | 1:101:A:ALA:H | 1:100:A:SER:HB3 | 3 | 0.38 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 8 | 0.38 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 6 | 0.38 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 6 | 0.38 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 6 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 4 | 0.38 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 4 | 0.38 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 9 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 8 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 8 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 8 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 9 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 9 | 0.38 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 9 | 0.38 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 2 | 0.38 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 10 | 0.38 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 9 | 0.38 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 9 | 0.38 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 9 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 1 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 1 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 1 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 2 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1910) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 2 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 3 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 3 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 3 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 5 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 5 | 0.38 |
| (1,1910) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 5 | 0.38 |
| (1,1898) | 1:115:A:VAL:H | 1:114:A:ARG:HG2 | 6 | 0.38 |
| (1,1896) | 1:114:A:ARG:HA | 1:114:A:ARG:HG2 | 10 | 0.38 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 4 | 0.38 |
| (1,1810) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD2 | 5 | 0.38 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 2 | 0.38 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 2 | 0.38 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 2 | 0.38 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD11 | 5 | 0.38 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD12 | 5 | 0.38 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD13 | 5 | 0.38 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 2 | 0.38 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 9 | 0.38 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 2 | 0.38 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 3 | 0.38 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 3 | 0.38 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 3 | 0.38 |
| (1,1560) | 1:92:A:GLU:HG3 | 1:93:A:SER:HB3 | 2 | 0.38 |
| (1,1532) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 8 | 0.38 |
| (1,1478) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HB3 | 1 | 0.38 |
| (1,1478) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HB3 | 1 | 0.38 |
| (1,1478) | 1:126:A:LEU:HD23 | 1:88:A:GLU:HB3 | 1 | 0.38 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 5 | 0.38 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 8 | 0.38 |
| (1,924) | 1:40:A:LYS:HE2 | 1:38:A:ILE:H | 1 | 0.38 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 9 | 0.38 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 9 | 0.38 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 9 | 0.38 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 2 | 0.38 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 2 | 0.38 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 2 | 0.38 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 1 | 0.38 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 1 | 0.38 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 1 | 0.38 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 5 | 0.38 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 5 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 5 | 0.38 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 3 | 0.38 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 3 | 0.38 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 3 | 0.38 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 9 | 0.38 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 9 | 0.38 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 9 | 0.38 |
| (1,25) | 1:7:A:ARG:HA | 1:7:A:ARG:HG2 | 4 | 0.38 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 2 | 0.37 |
| (3,1178) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 9 | 0.37 |
| (3,1157) | 1:80:A:LEU:HD12 | 1:14:A:TRP:HZ3 | 7 | 0.37 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 5 | 0.37 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 10 | 0.37 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 6 | 0.37 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 3 | 0.37 |
| (3,1020) | 1:110:A:LEU:HB2 | 1:110:A:LEU:HA | 10 | 0.37 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG21 | 7 | 0.37 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD3 | 1 | 0.37 |
| (3,751) | 1:43:A:ILE:HG21 | 1:43:A:ILE:H | 5 | 0.37 |
| (3,671) | 1:40:A:LYS:HB3 | 1:41:A:GLU:H | 1 | 0.37 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 4 | 0.37 |
| (3,568) | 1:19:A:ILE:HG21 | 1:78:A:LEU:HD13 | 4 | 0.37 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 2 | 0.37 |
| (3,345) | 1:35:A:LYS:H | 1:22:A:LYS:HG3 | 2 | 0.37 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD13 | 4 | 0.37 |
| (3,122) | 1:44:A:ASP:HB3 | 1:43:A:ILE:HG22 | 8 | 0.37 |
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD12 | 10 | 0.37 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 7 | 0.37 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 7 | 0.37 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 5 | 0.37 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 10 | 0.37 |
| (1,3641) | 1:11:A:THR:H | 1:81:A:ASN:HD21 | 7 | 0.37 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 2 | 0.37 |
| (1,3488) | 1:29:A:GLY:H | 1:32:A:TYR:HE1 | 6 | 0.37 |
| (1,3488) | 1:29:A:GLY:H | 1:32:A:TYR:HE2 | 6 | 0.37 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 10 | 0.37 |
| (1,3163) | 1:49:A:VAL:HG11 | 1:41:A:GLU:H | 3 | 0.37 |
| (1,3163) | 1:49:A:VAL:HG12 | 1:41:A:GLU:H | 3 | 0.37 |
| (1,3163) | 1:49:A:VAL:HG13 | 1:41:A:GLU:H | 3 | 0.37 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 3 | 0.37 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 3 | 0.37 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 3 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 6 | 0.37 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 9 | 0.37 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 10 | 0.37 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 5 | 0.37 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 9 | 0.37 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 3 | 0.37 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 9 | 0.37 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 2 | 0.37 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 10 | 0.37 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 4 | 0.37 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 4 | 0.37 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 4 | 0.37 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 10 | 0.37 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 2 | 0.37 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 8 | 0.37 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 8 | 0.37 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 8 | 0.37 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 5 | 0.37 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 3 | 0.37 |
| (1,1956) | 1:118:A:ILE:HD11 | 1:84:A:TYR:HD1 | 9 | 0.37 |
| (1,1956) | 1:118:A:ILE:HD11 | 1:84:A:TYR:HD2 | 9 | 0.37 |
| (1,1956) | 1:118:A:ILE:HD12 | 1:84:A:TYR:HD1 | 9 | 0.37 |
| (1,1956) | 1:118:A:ILE:HD12 | 1:84:A:TYR:HD2 | 9 | 0.37 |
| (1,1956) | 1:118:A:ILE:HD13 | 1:84:A:TYR:HD1 | 9 | 0.37 |
| (1,1956) | 1:118:A:ILE:HD13 | 1:84:A:TYR:HD2 | 9 | 0.37 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 5 | 0.37 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 8 | 0.37 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 10 | 0.37 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 9 | 0.37 |
| (1,1910) | 1:115:A:VAL:HG11 | 1:115:A:VAL:HA | 7 | 0.37 |
| (1,1910) | 1:115:A:VAL:HG12 | 1:115:A:VAL:HA | 7 | 0.37 |
| (1,1910) | 1:115:A:VAL:HG13 | 1:115:A:VAL:HA | 7 | 0.37 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 2 | 0.37 |
| (1,1823) | 1:110:A:LEU:H | 1:109:A:PRO:HG2 | 6 | 0.37 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 6 | 0.37 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 6 | 0.37 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 6 | 0.37 |
| (1,1608) | 1:97:A:LYS:HG2 | 1:97:A:LYS:HA | 5 | 0.37 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 5 | 0.37 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 5 | 0.37 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 4 | 0.37 |
| (1,1262) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 3 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1258) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 5 | 0.37 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB1 | 5 | 0.37 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB2 | 5 | 0.37 |
| (1,1215) | 1:75:A:LYS:HE3 | 1:72:A:ALA:HB3 | 5 | 0.37 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 2 | 0.37 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 10 | 0.37 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 4 | 0.37 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 4 | 0.37 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 4 | 0.37 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 3 | 0.37 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE1 | 3 | 0.37 |
| (1,836) | 1:52:A:MET:HG2 | 1:32:A:TYR:HE2 | 3 | 0.37 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 1 | 0.37 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 1 | 0.37 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 6 | 0.37 |
| (1,693) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 10 | 0.37 |
| (1,693) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 10 | 0.37 |
| (1,693) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 10 | 0.37 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 7 | 0.37 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 7 | 0.37 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 7 | 0.37 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 10 | 0.37 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 10 | 0.37 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 10 | 0.37 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 7 | 0.37 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 7 | 0.37 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 7 | 0.37 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 10 | 0.37 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 3 | 0.37 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 3 | 0.37 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 3 | 0.37 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 1 | 0.37 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 1 | 0.37 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 1 | 0.37 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 5 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 5 | 0.37 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 5 | 0.37 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 3 | 0.37 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 3 | 0.37 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 3 | 0.37 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 7 | 0.37 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 7 | 0.37 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 7 | 0.37 |
| (3,1221) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HD11 | 9 | 0.36 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HG2 | 1 | 0.36 |
| (3,1156) | 1:10:A:ARG:HG2 | 1:10:A:ARG:H | 2 | 0.36 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 9 | 0.36 |
| (3,1091) | 1:112:A:GLY:H | 1:105:A:ILE:H | 3 | 0.36 |
| (3,1087) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HB3 | 1 | 0.36 |
| (3,1087) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HB3 | 1 | 0.36 |
| (3,1087) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HB3 | 1 | 0.36 |
| (3,1076) | 1:97:A:LYS:H | 1:97:A:LYS:HD3 | 9 | 0.36 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 5 | 0.36 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 1 | 0.36 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 2 | 0.36 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG22 | 7 | 0.36 |
| (3,876) | 1:10:A:ARG:HD3 | 1:81:A:ASN:HD21 | 8 | 0.36 |
| (3,782) | 1:96:A:GLU:HB3 | 1:94:A:ILE:HD11 | 6 | 0.36 |
| (3,782) | 1:96:A:GLU:HB3 | 1:94:A:ILE:HD12 | 6 | 0.36 |
| (3,782) | 1:96:A:GLU:HB3 | 1:94:A:ILE:HD13 | 6 | 0.36 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD12 | 2 | 0.36 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 10 | 0.36 |
| (3,751) | 1:43:A:ILE:HG23 | 1:43:A:ILE:H | 6 | 0.36 |
| (3,751) | 1:43:A:ILE:HG21 | 1:43:A:ILE:H | 9 | 0.36 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 2 | 0.36 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 5 | 0.36 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 6 | 0.36 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 9 | 0.36 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG23 | 1 | 0.36 |
| (3,537) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 8 | 0.36 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 9 | 0.36 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 2 | 0.36 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 5 | 0.36 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 1 | 0.36 |
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 7 | 0.36 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 10 | 0.36 |
| (3,125) | 1:44:A:ASP:HB2 | 1:46:A:TYR:HD1 | 8 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,30) | 1:103:A:ILE:H | 1:103:A:ILE:HD12 | 6 | 0.36 |
| (3,4) | 1:102:A:THR:HG23 | 1:116:A:GLU:H | 6 | 0.36 |
| (2,142) | 1:10:A:ARG:HA | 1:82:A:GLY:HA3 | 10 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD11 | 3 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD12 | 3 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD13 | 3 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD11 | 3 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD12 | 3 | 0.36 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD13 | 3 | 0.36 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 1 | 0.36 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 1 | 0.36 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 1 | 0.36 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 1 | 0.36 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 7 | 0.36 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 4 | 0.36 |
| (1,3557) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HD21 | 7 | 0.36 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 2 | 0.36 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 10 | 0.36 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 1 | 0.36 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 1 | 0.36 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 1 | 0.36 |
| (1,3245) | 1:30:A:GLU:HG2 | 1:33:A:HIS:H | 2 | 0.36 |
| (1,3163) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 4 | 0.36 |
| (1,3163) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 4 | 0.36 |
| (1,3163) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 4 | 0.36 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 3 | 0.36 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 3 | 0.36 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 3 | 0.36 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 10 | 0.36 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 8 | 0.36 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 7 | 0.36 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 7 | 0.36 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 7 | 0.36 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 3 | 0.36 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 3 | 0.36 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 2 | 0.36 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 4 | 0.36 |
| (1,2287) | 1:20:A:ILE:HA | 1:38:A:ILE:HG13 | 10 | 0.36 |
| (1,2183) | 1:111:A:LYS:HE2 | 1:111:A:LYS:HA | 6 | 0.36 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 5 | 0.36 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 1 | 0.36 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 1 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 1 | 0.36 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 2 | 0.36 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 2 | 0.36 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 2 | 0.36 |
| (1,1953) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 4 | 0.36 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 5 | 0.36 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 5 | 0.36 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 1 | 0.36 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 1 | 0.36 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 1 | 0.36 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 10 | 0.36 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 10 | 0.36 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 10 | 0.36 |
| (1,1640) | 1:119:A:GLN:HA | 1:100:A:SER:HB2 | 9 | 0.36 |
| (1,1638) | 1:118:A:ILE:H | 1:100:A:SER:HB2 | 5 | 0.36 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 8 | 0.36 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 6 | 0.36 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG21 | 10 | 0.36 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG22 | 10 | 0.36 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG23 | 10 | 0.36 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 3 | 0.36 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 3 | 0.36 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 3 | 0.36 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 2 | 0.36 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 2 | 0.36 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 2 | 0.36 |
| (1,781) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 10 | 0.36 |
| (1,781) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 10 | 0.36 |
| (1,781) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 10 | 0.36 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 7 | 0.36 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 7 | 0.36 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 2 | 0.36 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 2 | 0.36 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 2 | 0.36 |
| (3,1181) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 9 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,1178) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HG2 | 7 | 0.35 |
| (3,1093) | 1:70:A:ILE:HD12 | 1:123:A:ILE:H | 5 | 0.35 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 10 | 0.35 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG23 | 2 | 0.35 |
| (3,951) | 1:80:A:LEU:HD13 | 1:124:A:SER:H | 4 | 0.35 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 9 | 0.35 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 3 | 0.35 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 6 | 0.35 |
| (3,751) | 1:43:A:ILE:HG22 | 1:43:A:ILE:H | 2 | 0.35 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 10 | 0.35 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG22 | 9 | 0.35 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 2 | 0.35 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 9 | 0.35 |
| (3,600) | 1:54:A:ASP:H | 1:53:A:ILE:HG13 | 3 | 0.35 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 3 | 0.35 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 1 | 0.35 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 7 | 0.35 |
| (3,280) | 1:112:A:GLY:H | 1:111:A:LYS:HG3 | 10 | 0.35 |
| (3,158) | 1:76:A:ARG:HG3 | 1:91:A:LEU:H | 10 | 0.35 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 3 | 0.35 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 3 | 0.35 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 2 | 0.35 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD11 | 3 | 0.35 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD12 | 3 | 0.35 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD13 | 3 | 0.35 |
| (1,3726) | 1:95:A:ASN:HD21 | 1:98:A:THR:HB | 5 | 0.35 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 4 | 0.35 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 8 | 0.35 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 5 | 0.35 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 5 | 0.35 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 5 | 0.35 |
| (1,3411) | 1:3:A:GLU:HG3 | 1:3:A:GLU:H | 3 | 0.35 |
| (1,3403) | 1:10:A:ARG:HD2 | 1:10:A:ARG:H | 1 | 0.35 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 7 | 0.35 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 7 | 0.35 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 7 | 0.35 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 3 | 0.35 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 2 | 0.35 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE1 | 10 | 0.35 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE2 | 10 | 0.35 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 1 | 0.35 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 7 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 10 | 0.35 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 8 | 0.35 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 9 | 0.35 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 9 | 0.35 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 8 | 0.35 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 8 | 0.35 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 8 | 0.35 |
| (1,2709) | 1:103:A:ILE:HB | 1:89:A:GLY:H | 7 | 0.35 |
| (1,2687) | 1:91:A:LEU:H | 1:91:A:LEU:HB3 | 6 | 0.35 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 5 | 0.35 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 9 | 0.35 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 2 | 0.35 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 5 | 0.35 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 6 | 0.35 |
| (1,2128) | 1:70:A:ILE:HD11 | 1:121:A:GLU:HA | 10 | 0.35 |
| (1,2128) | 1:70:A:ILE:HD12 | 1:121:A:GLU:HA | 10 | 0.35 |
| (1,2128) | 1:70:A:ILE:HD13 | 1:121:A:GLU:HA | 10 | 0.35 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 5 | 0.35 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 5 | 0.35 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 5 | 0.35 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 6 | 0.35 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 6 | 0.35 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 6 | 0.35 |
| (1,2047) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 9 | 0.35 |
| (1,2047) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 9 | 0.35 |
| (1,2047) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 9 | 0.35 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 2 | 0.35 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 2 | 0.35 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 2 | 0.35 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 8 | 0.35 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 5 | 0.35 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 5 | 0.35 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 5 | 0.35 |
| (1,1370) | 1:122:A:ASP:HA | 1:80:A:LEU:HB3 | 1 | 0.35 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 4 | 0.35 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 5 | 0.35 |
| (1,1258) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 8 | 0.35 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 6 | 0.35 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 2 | 0.35 |
| (1,959) | 1:60:A:LYS:HD2 | 1:61:A:LEU:H | 7 | 0.35 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 4 | 0.35 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 6 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 6 | 0.35 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 6 | 0.35 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 6 | 0.35 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 6 | 0.35 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 6 | 0.35 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 9 | 0.35 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 3 | 0.35 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 3 | 0.35 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 3 | 0.35 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 7 | 0.35 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 7 | 0.35 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 7 | 0.35 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 6 | 0.35 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 6 | 0.35 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 6 | 0.35 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 1 | 0.35 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 2 | 0.35 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 2 | 0.35 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 2 | 0.35 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 10 | 0.35 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 10 | 0.35 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 10 | 0.35 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 6 | 0.35 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 6 | 0.35 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 6 | 0.35 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 9 | 0.35 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 9 | 0.35 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 9 | 0.35 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 8 | 0.34 |
| (3,1157) | 1:80:A:LEU:HD11 | 1:14:A:TRP:HZ3 | 4 | 0.34 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 3 | 0.34 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 6 | 0.34 |
| (3,973) | 1:20:A:ILE:HG22 | 1:21:A:VAL:H | 2 | 0.34 |
| (3,849) | 1:35:A:LYS:HD2 | 1:33:A:HIS:H | 4 | 0.34 |
| (3,849) | 1:35:A:LYS:HD2 | 1:33:A:HIS:H | 9 | 0.34 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 7 | 0.34 |
| (3,732) | 1:48:A:ALA:HB2 | 1:43:A:ILE:H | 4 | 0.34 |
| (3,732) | 1:43:A:ILE:H | 1:43:A:ILE:HG12 | 7 | 0.34 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 2 | 0.34 |
| (3,537) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 3 | 0.34 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 4 | 0.34 |
| (3,296) | 1:91:A:LEU:HD22 | 1:91:A:LEU:HG | 7 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,293) | 1:27:A:LYS:HG3 | 1:27:A:LYS:HA | 5 | 0.34 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 10 | 0.34 |
| (3,165) | 1:79:A:VAL:HG11 | 1:88:A:GLU:HA | 9 | 0.34 |
| (3,43) | 1:77:A:ILE:H | 1:77:A:ILE:HG22 | 6 | 0.34 |
| (3,23) | 1:127:A:ALA:HB3 | 1:18:A:GLU:H | 9 | 0.34 |
| (3,4) | 1:102:A:THR:HG22 | 1:116:A:GLU:H | 8 | 0.34 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD11 | 5 | 0.34 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD12 | 5 | 0.34 |
| (2,419) | 1:22:A:LYS:HE2 | 1:24:A:ILE:HD13 | 5 | 0.34 |
| (2,338) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG12 | 9 | 0.34 |
| (1,3737) | 1:5:A:LYS:H | 1:3:A:GLU:H | 6 | 0.34 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 7 | 0.34 |
| (1,3631) | 1:23:A:ILE:H | 1:32:A:TYR:HB3 | 10 | 0.34 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 9 | 0.34 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 8 | 0.34 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 6 | 0.34 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 6 | 0.34 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 6 | 0.34 |
| (1,3449) | 1:15:A:LEU:H | 1:14:A:TRP:HE1 | 10 | 0.34 |
| (1,3414) | 1:4:A:GLU:H | 1:3:A:GLU:H | 6 | 0.34 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 5 | 0.34 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 5 | 0.34 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 5 | 0.34 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 9 | 0.34 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 7 | 0.34 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 7 | 0.34 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 7 | 0.34 |
| (1,3018) | 1:52:A:MET:HG2 | 1:57:A:ASP:H | 1 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 2 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 3 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 4 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 5 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 6 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 8 | 0.34 |
| (1,2969) | 1:63:A:GLN:H | 1:63:A:GLN:HB2 | 9 | 0.34 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 5 | 0.34 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 3 | 0.34 |
| (1,2517) | 1:88:A:GLU:HB2 | 1:106:A:GLU:H | 1 | 0.34 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 3 | 0.34 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 3 | 0.34 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 3 | 0.34 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 8 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 8 | 0.34 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 8 | 0.34 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 7 | 0.34 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 10 | 0.34 |
| (1,2304) | 1:104:A:VAL:HG21 | 1:114:A:ARG:HB3 | 10 | 0.34 |
| (1,2304) | 1:104:A:VAL:HG22 | 1:114:A:ARG:HB3 | 10 | 0.34 |
| (1,2304) | 1:104:A:VAL:HG23 | 1:114:A:ARG:HB3 | 10 | 0.34 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 7 | 0.34 |
| (1,2221) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HA | 1 | 0.34 |
| (1,2221) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HA | 1 | 0.34 |
| (1,2221) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 1 | 0.34 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 1 | 0.34 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 1 | 0.34 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 1 | 0.34 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 1 | 0.34 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 1 | 0.34 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 1 | 0.34 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 7 | 0.34 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 8 | 0.34 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 8 | 0.34 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 8 | 0.34 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 7 | 0.34 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 7 | 0.34 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 7 | 0.34 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 4 | 0.34 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 8 | 0.34 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 3 | 0.34 |
| (1,1262) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 5 | 0.34 |
| (1,1258) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 7 | 0.34 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 6 | 0.34 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 6 | 0.34 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 6 | 0.34 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 8 | 0.34 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 6 | 0.34 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 6 | 0.34 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 6 | 0.34 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 3 | 0.34 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 7 | 0.34 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 9 | 0.34 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 9 | 0.34 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 9 | 0.34 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 9 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 9 | 0.34 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 9 | 0.34 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 9 | 0.34 |
| (1,851) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HB | 6 | 0.34 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 5 | 0.34 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 5 | 0.34 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 10 | 0.34 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 10 | 0.34 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 10 | 0.34 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 2 | 0.34 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 2 | 0.34 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 4 | 0.34 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 4 | 0.34 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 4 | 0.34 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 7 | 0.34 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 7 | 0.34 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 7 | 0.34 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 7 | 0.34 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 7 | 0.34 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 7 | 0.34 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 8 | 0.34 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 8 | 0.34 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 8 | 0.34 |
| (1,375) | 1:23:A:ILE:HG21 | 1:66:A:LEU:HA | 5 | 0.34 |
| (1,375) | 1:23:A:ILE:HG22 | 1:66:A:LEU:HA | 5 | 0.34 |
| (1,375) | 1:23:A:ILE:HG23 | 1:66:A:LEU:HA | 5 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 1 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 1 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 1 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 3 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 3 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 3 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 4 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 4 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 4 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 6 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 6 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 6 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 7 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 7 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 7 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 8 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 8 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 8 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 9 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 9 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 9 | 0.34 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 10 | 0.34 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 10 | 0.34 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 10 | 0.34 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD11 | 9 | 0.34 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD12 | 9 | 0.34 |
| (1,201) | 1:73:A:PRO:HG2 | 1:91:A:LEU:HD13 | 9 | 0.34 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 4 | 0.34 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 4 | 0.34 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 4 | 0.34 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 9 | 0.34 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 9 | 0.34 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 9 | 0.34 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 2 | 0.34 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 2 | 0.34 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 2 | 0.34 |
| (1,25) | 1:7:A:ARG:HA | 1:7:A:ARG:HG2 | 5 | 0.34 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 6 | 0.33 |
| (3,1087) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HB3 | 4 | 0.33 |
| (3,1087) | 1:61:A:LEU:HD12 | 1:59:A:LEU:HB3 | 4 | 0.33 |
| (3,1087) | 1:61:A:LEU:HD13 | 1:59:A:LEU:HB3 | 4 | 0.33 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 5 | 0.33 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 7 | 0.33 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 8 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,995) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 3 | 0.33 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG22 | 4 | 0.33 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD11 | 1 | 0.33 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 1 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 1 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 2 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 3 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 4 | 0.33 |
| (3,843) | 1:75:A:LYS:HB2 | 1:75:A:LYS:HA | 5 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 6 | 0.33 |
| (3,843) | 1:75:A:LYS:HB2 | 1:75:A:LYS:HA | 7 | 0.33 |
| (3,843) | 1:75:A:LYS:HB2 | 1:75:A:LYS:HA | 8 | 0.33 |
| (3,843) | 1:40:A:LYS:HA | 1:40:A:LYS:HB2 | 9 | 0.33 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG22 | 3 | 0.33 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD2 | 5 | 0.33 |
| (3,722) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 3 | 0.33 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 1 | 0.33 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 5 | 0.33 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 10 | 0.33 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 9 | 0.33 |
| (3,595) | 1:105:A:ILE:HB | 1:106:A:GLU:H | 7 | 0.33 |
| (3,533) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB3 | 3 | 0.33 |
| (3,489) | 1:82:A:GLY:HA3 | 1:81:A:ASN:HB3 | 7 | 0.33 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 8 | 0.33 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 8 | 0.33 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 9 | 0.33 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 3 | 0.33 |
| (3,153) | 1:91:A:LEU:HD11 | 1:102:A:THR:H | 1 | 0.33 |
| (3,69) | 1:66:A:LEU:HD11 | 1:21:A:VAL:HB | 10 | 0.33 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 2 | 0.33 |
| (2,591) | 1:11:A:THR:H | 1:13:A:TYR:HD1 | 4 | 0.33 |
| (2,591) | 1:11:A:THR:H | 1:13:A:TYR:HD2 | 4 | 0.33 |
| (2,589) | 1:82:A:GLY:HA3 | 1:11:A:THR:H | 1 | 0.33 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 6 | 0.33 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 2 | 0.33 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 2 | 0.33 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 2 | 0.33 |
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 3 | 0.33 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 1 | 0.33 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 10 | 0.33 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 10 | 0.33 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 8 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 10 | 0.33 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 10 | 0.33 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 10 | 0.33 |
| (1,3453) | 1:14:A:TRP:HA | 1:16:A:GLN:HE22 | 8 | 0.33 |
| (1,3414) | 1:4:A:GLU:H | 1:3:A:GLU:H | 3 | 0.33 |
| (1,3402) | 1:9:A:ALA:HA | 1:10:A:ARG:H | 5 | 0.33 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 7 | 0.33 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 7 | 0.33 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 7 | 0.33 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 2 | 0.33 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 6 | 0.33 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 8 | 0.33 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 8 | 0.33 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 8 | 0.33 |
| (1,3163) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 10 | 0.33 |
| (1,3163) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 10 | 0.33 |
| (1,3163) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 10 | 0.33 |
| (1,3128) | 1:47:A:THR:HB | 1:44:A:ASP:H | 5 | 0.33 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 5 | 0.33 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE1 | 9 | 0.33 |
| (1,3063) | 1:52:A:MET:H | 1:32:A:TYR:HE2 | 9 | 0.33 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 3 | 0.33 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 3 | 0.33 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 3 | 0.33 |
| (1,2848) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 7 | 0.33 |
| (1,2788) | 1:81:A:ASN:H | 1:84:A:TYR:H | 1 | 0.33 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 10 | 0.33 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 10 | 0.33 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 10 | 0.33 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 6 | 0.33 |
| (1,2584) | 1:100:A:SER:H | 1:119:A:GLN:HE22 | 8 | 0.33 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 6 | 0.33 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 2 | 0.33 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 2 | 0.33 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 2 | 0.33 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 4 | 0.33 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 4 | 0.33 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 8 | 0.33 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 9 | 0.33 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 6 | 0.33 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 6 | 0.33 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 6 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2205) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 5 | 0.33 |
| (1,2205) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 5 | 0.33 |
| (1,2205) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 5 | 0.33 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 2 | 0.33 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 2 | 0.33 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 2 | 0.33 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 2 | 0.33 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 2 | 0.33 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 2 | 0.33 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 2 | 0.33 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 1 | 0.33 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 1 | 0.33 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 1 | 0.33 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 4 | 0.33 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 5 | 0.33 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 3 | 0.33 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 3 | 0.33 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 3 | 0.33 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 3 | 0.33 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 6 | 0.33 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 10 | 0.33 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 5 | 0.33 |
| (1,965) | 1:22:A:LYS:HE2 | 1:22:A:LYS:HG2 | 8 | 0.33 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 3 | 0.33 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 3 | 0.33 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 3 | 0.33 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 3 | 0.33 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 3 | 0.33 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 3 | 0.33 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 3 | 0.33 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 10 | 0.33 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 10 | 0.33 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 10 | 0.33 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 1 | 0.33 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 1 | 0.33 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 1 | 0.33 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 8 | 0.33 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD11 | 7 | 0.33 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD12 | 7 | 0.33 |
| (1,686) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HD13 | 7 | 0.33 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 7 | 0.33 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 7 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 7 | 0.33 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 8 | 0.33 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 8 | 0.33 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 8 | 0.33 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 2 | 0.33 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 2 | 0.33 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 2 | 0.33 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 1 | 0.33 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 1 | 0.33 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 1 | 0.33 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 5 | 0.33 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 5 | 0.33 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 5 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 1 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 1 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 1 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 5 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 5 | 0.33 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 5 | 0.33 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD11 | 1 | 0.33 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD12 | 1 | 0.33 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD13 | 1 | 0.33 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 2 | 0.33 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 2 | 0.33 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 2 | 0.33 |
| (1,311) | 1:21:A:VAL:HG21 | 1:21:A:VAL:HA | 5 | 0.33 |
| (1,311) | 1:21:A:VAL:HG22 | 1:21:A:VAL:HA | 5 | 0.33 |
| (1,311) | 1:21:A:VAL:HG23 | 1:21:A:VAL:HA | 5 | 0.33 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 4 | 0.33 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 4 | 0.33 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 4 | 0.33 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 8 | 0.33 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 8 | 0.33 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 8 | 0.33 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 5 | 0.33 |
| (3,1210) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG23 | 10 | 0.32 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 1 | 0.32 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 3 | 0.32 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 4 | 0.32 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG21 | 6 | 0.32 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 8 | 0.32 |
| (3,1030) | 1:53:A:ILE:H | 1:37:A:ALA:H | 7 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 8 | 0.32 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG22 | 8 | 0.32 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 6 | 0.32 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD13 | 5 | 0.32 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD11 | 4 | 0.32 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 4 | 0.32 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 8 | 0.32 |
| (3,595) | 1:105:A:ILE:HB | 1:106:A:GLU:H | 1 | 0.32 |
| (3,568) | 1:19:A:ILE:HG21 | 1:78:A:LEU:HD11 | 2 | 0.32 |
| (3,423) | 1:61:A:LEU:HD12 | 1:25:A:THR:H | 8 | 0.32 |
| (3,348) | 1:7:A:ARG:HD2 | 1:7:A:ARG:H | 10 | 0.32 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 4 | 0.32 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 6 | 0.32 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 10 | 0.32 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG21 | 3 | 0.32 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD11 | 5 | 0.32 |
| (3,125) | 1:13:A:TYR:HD2 | 1:45:A:LYS:HE3 | 2 | 0.32 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 10 | 0.32 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 7 | 0.32 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG11 | 8 | 0.32 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG12 | 8 | 0.32 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG13 | 8 | 0.32 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 8 | 0.32 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 8 | 0.32 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD1 | 1 | 0.32 |
| (1,3780) | 1:63:A:GLN:HB2 | 1:46:A:TYR:HD2 | 1 | 0.32 |
| (1,3777) | 1:45:A:LYS:HG2 | 1:46:A:TYR:HD1 | 9 | 0.32 |
| (1,3777) | 1:45:A:LYS:HG2 | 1:46:A:TYR:HD2 | 9 | 0.32 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 5 | 0.32 |
| (1,3652) | 1:22:A:LYS:H | 1:22:A:LYS:HE2 | 3 | 0.32 |
| (1,3599) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD22 | 8 | 0.32 |
| (1,3599) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD22 | 8 | 0.32 |
| (1,3599) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD22 | 8 | 0.32 |
| (1,3475) | 1:19:A:ILE:HD11 | 1:18:A:GLU:H | 1 | 0.32 |
| (1,3475) | 1:19:A:ILE:HD12 | 1:18:A:GLU:H | 1 | 0.32 |
| (1,3475) | 1:19:A:ILE:HD13 | 1:18:A:GLU:H | 1 | 0.32 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 6 | 0.32 |
| (1,3444) | 1:63:A:GLN:HB3 | 1:14:A:TRP:HE1 | 8 | 0.32 |
| (1,3322) | 1:22:A:LYS:H | 1:67:A:GLU:HB2 | 5 | 0.32 |
| (1,3245) | 1:30:A:GLU:HG2 | 1:33:A:HIS:H | 1 | 0.32 |
| (1,3245) | 1:30:A:GLU:HG3 | 1:33:A:HIS:H | 5 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD11 | 1 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD12 | 1 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD13 | 1 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD11 | 3 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD12 | 3 | 0.32 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD13 | 3 | 0.32 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 6 | 0.32 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 1 | 0.32 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 1 | 0.32 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 1 | 0.32 |
| (1,3126) | 1:44:A:ASP:H | 1:47:A:THR:HA | 9 | 0.32 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 5 | 0.32 |
| (1,2863) | 1:75:A:LYS:HB2 | 1:75:A:LYS:H | 10 | 0.32 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 8 | 0.32 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 6 | 0.32 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 9 | 0.32 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 4 | 0.32 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 7 | 0.32 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 7 | 0.32 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 7 | 0.32 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 4 | 0.32 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 1 | 0.32 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 3 | 0.32 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 3 | 0.32 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 3 | 0.32 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 3 | 0.32 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 10 | 0.32 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 10 | 0.32 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 10 | 0.32 |
| (1,2256) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HB | 5 | 0.32 |
| (1,2243) | 1:52:A:MET:HB3 | 1:55:A:SER:HB2 | 10 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 1 | 0.32 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 1 | 0.32 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 3 | 0.32 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 3 | 0.32 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 3 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 3 | 0.32 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 3 | 0.32 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 3 | 0.32 |
| (1,2205) | 1:49:A:VAL:HG11 | 1:41:A:GLU:H | 3 | 0.32 |
| (1,2205) | 1:49:A:VAL:HG12 | 1:41:A:GLU:H | 3 | 0.32 |
| (1,2205) | 1:49:A:VAL:HG13 | 1:41:A:GLU:H | 3 | 0.32 |
| (1,2168) | 1:61:A:LEU:HG | 1:65:A:HIS:HB3 | 1 | 0.32 |
| (1,2158) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 5 | 0.32 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 4 | 0.32 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 2 | 0.32 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 2 | 0.32 |
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 2 | 0.32 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 5 | 0.32 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 2 | 0.32 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 9 | 0.32 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 9 | 0.32 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 9 | 0.32 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 6 | 0.32 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 6 | 0.32 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 6 | 0.32 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 8 | 0.32 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 7 | 0.32 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 7 | 0.32 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 7 | 0.32 |
| (1,1262) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 8 | 0.32 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 1 | 0.32 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 5 | 0.32 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 2 | 0.32 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 2 | 0.32 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 2 | 0.32 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 2 | 0.32 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 2 | 0.32 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 2 | 0.32 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 8 | 0.32 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 8 | 0.32 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 9 | 0.32 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 1 | 0.32 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 1 | 0.32 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 1 | 0.32 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 9 | 0.32 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 9 | 0.32 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 9 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 9 | 0.32 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 9 | 0.32 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 9 | 0.32 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 9 | 0.32 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 9 | 0.32 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 9 | 0.32 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 4 | 0.32 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HG2 | 7 | 0.31 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 2 | 0.31 |
| (3,1142) | 1:109:A:PRO:HB2 | 1:109:A:PRO:HD3 | 9 | 0.31 |
| (3,993) | 1:61:A:LEU:HG | 1:50:A:VAL:H | 2 | 0.31 |
| (3,865) | 1:31:A:LYS:HG2 | 1:31:A:LYS:HE2 | 4 | 0.31 |
| (3,865) | 1:31:A:LYS:HG2 | 1:31:A:LYS:HE2 | 8 | 0.31 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 6 | 0.31 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD13 | 3 | 0.31 |
| (3,743) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HA | 6 | 0.31 |
| (3,743) | 1:37:A:ALA:HB2 | 1:50:A:VAL:HA | 10 | 0.31 |
| (3,640) | 1:120:A:TYR:HA | 1:120:A:TYR:H | 3 | 0.31 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD11 | 2 | 0.31 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD11 | 5 | 0.31 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD12 | 7 | 0.31 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 4 | 0.31 |
| (3,537) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 4 | 0.31 |
| (3,423) | 1:61:A:LEU:HD13 | 1:25:A:THR:H | 1 | 0.31 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 5 | 0.31 |
| (3,348) | 1:113:A:ARG:H | 1:113:A:ARG:HD2 | 6 | 0.31 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 8 | 0.31 |
| (3,300) | 1:11:A:THR:HG21 | 1:13:A:TYR:HE1 | 1 | 0.31 |
| (3,296) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 2 | 0.31 |
| (3,296) | 1:91:A:LEU:HD23 | 1:91:A:LEU:HG | 10 | 0.31 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 7 | 0.31 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 8 | 0.31 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 1 | 0.31 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 2 | 0.31 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 4 | 0.31 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 7 | 0.31 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 9 | 0.31 |
| (3,165) | 1:79:A:VAL:HG13 | 1:88:A:GLU:HA | 8 | 0.31 |
| (3,153) | 1:123:A:ILE:HD13 | 1:102:A:THR:H | 2 | 0.31 |
| (3,85) | 1:36:A:LYS:HA | 1:69:A:VAL:HG12 | 10 | 0.31 |
| (2,574) | 1:39:A:VAL:H | 1:20:A:ILE:HG12 | 6 | 0.31 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG11 | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG12 | 10 | 0.31 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG13 | 10 | 0.31 |
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 5 | 0.31 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 4 | 0.31 |
| (1,3715) | 1:84:A:TYR:HE1 | 1:87:A:ASN:HD22 | 5 | 0.31 |
| (1,3715) | 1:84:A:TYR:HE2 | 1:87:A:ASN:HD22 | 5 | 0.31 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 9 | 0.31 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 6 | 0.31 |
| (1,3415) | 1:7:A:ARG:HG3 | 1:7:A:ARG:H | 8 | 0.31 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 9 | 0.31 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 9 | 0.31 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 9 | 0.31 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 4 | 0.31 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 4 | 0.31 |
| (1,3000) | 1:59:A:LEU:HD11 | 1:60:A:LYS:H | 10 | 0.31 |
| (1,3000) | 1:59:A:LEU:HD12 | 1:60:A:LYS:H | 10 | 0.31 |
| (1,3000) | 1:59:A:LEU:HD13 | 1:60:A:LYS:H | 10 | 0.31 |
| (1,2921) | 1:21:A:VAL:HG21 | 1:67:A:GLU:H | 8 | 0.31 |
| (1,2921) | 1:21:A:VAL:HG22 | 1:67:A:GLU:H | 8 | 0.31 |
| (1,2921) | 1:21:A:VAL:HG23 | 1:67:A:GLU:H | 8 | 0.31 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 6 | 0.31 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 9 | 0.31 |
| (1,2641) | 1:95:A:ASN:HD21 | 1:95:A:ASN:H | 2 | 0.31 |
| (1,2633) | 1:96:A:GLU:H | 1:95:A:ASN:HB3 | 4 | 0.31 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 9 | 0.31 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 1 | 0.31 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 4 | 0.31 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 7 | 0.31 |
| (1,2346) | 1:124:A:SER:H | 1:78:A:LEU:HB2 | 7 | 0.31 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 5 | 0.31 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 5 | 0.31 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 5 | 0.31 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 8 | 0.31 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 8 | 0.31 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 8 | 0.31 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 4 | 0.31 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 4 | 0.31 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 4 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 4 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 4 | 0.31 |
| (1,2205) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 4 | 0.31 |
| (1,2193) | 1:107:A:THR:HG21 | 1:87:A:ASN:HA | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2193) | 1:107:A:THR:HG22 | 1:87:A:ASN:HA | 10 | 0.31 |
| (1,2193) | 1:107:A:THR:HG23 | 1:87:A:ASN:HA | 10 | 0.31 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 2 | 0.31 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 3 | 0.31 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 3 | 0.31 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 3 | 0.31 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 5 | 0.31 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 5 | 0.31 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 8 | 0.31 |
| (1,1608) | 1:97:A:LYS:HG2 | 1:97:A:LYS:HA | 8 | 0.31 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 9 | 0.31 |
| (1,1262) | 1:75:A:LYS:HD2 | 1:75:A:LYS:HA | 7 | 0.31 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 2 | 0.31 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 2 | 0.31 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 2 | 0.31 |
| (1,1220) | 1:73:A:PRO:HA | 1:91:A:LEU:HB2 | 9 | 0.31 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 8 | 0.31 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 8 | 0.31 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 8 | 0.31 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 6 | 0.31 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 8 | 0.31 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG21 | 6 | 0.31 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG22 | 6 | 0.31 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG23 | 6 | 0.31 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 1 | 0.31 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 4 | 0.31 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 10 | 0.31 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 3 | 0.31 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 10 | 0.31 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 2 | 0.31 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 5 | 0.31 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 5 | 0.31 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 5 | 0.31 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 7 | 0.31 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 7 | 0.31 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 7 | 0.31 |
| (1,683) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HA | 7 | 0.31 |
| (1,683) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HA | 7 | 0.31 |
| (1,683) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HA | 7 | 0.31 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 6 | 0.31 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 6 | 0.31 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 6 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 9 | 0.31 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 9 | 0.31 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 9 | 0.31 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 3 | 0.31 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 3 | 0.31 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 3 | 0.31 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 3 | 0.31 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 8 | 0.31 |
| (1,434) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 8 | 0.31 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 2 | 0.31 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 2 | 0.31 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 2 | 0.31 |
| (1,25) | 1:7:A:ARG:HA | 1:7:A:ARG:HG2 | 10 | 0.31 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 3 | 0.31 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 5 | 0.31 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 9 | 0.31 |
| (3,1182) | 1:118:A:ILE:HG22 | 1:118:A:ILE:HA | 4 | 0.3 |
| (3,1182) | 1:118:A:ILE:HG22 | 1:118:A:ILE:HA | 6 | 0.3 |
| (3,1178) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HG2 | 8 | 0.3 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HG2 | 6 | 0.3 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 1 | 0.3 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 2 | 0.3 |
| (3,1128) | 1:72:A:ALA:H | 1:71:A:PRO:HB3 | 7 | 0.3 |
| (3,1128) | 1:75:A:LYS:HG2 | 1:72:A:ALA:H | 9 | 0.3 |
| (3,1060) | 1:9:A:ALA:HB2 | 1:9:A:ALA:H | 7 | 0.3 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 6 | 0.3 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 9 | 0.3 |
| (3,1025) | 1:102:A:THR:H | 1:103:A:ILE:H | 10 | 0.3 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 3 | 0.3 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 9 | 0.3 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 1 | 0.3 |
| (3,885) | 1:69:A:VAL:HG21 | 1:69:A:VAL:HB | 4 | 0.3 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 2 | 0.3 |
| (3,789) | 1:118:A:ILE:HG12 | 1:101:A:ALA:H | 6 | 0.3 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD11 | 7 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,735) | 1:115:A:VAL:HG11 | 1:103:A:ILE:HD13 | 2 | 0.3 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 9 | 0.3 |
| (3,634) | 1:77:A:ILE:HG12 | 1:104:A:VAL:H | 3 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD12 | 3 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD11 | 4 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD13 | 6 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD13 | 8 | 0.3 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD13 | 10 | 0.3 |
| (3,440) | 1:93:A:SER:H | 1:103:A:ILE:H | 2 | 0.3 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 4 | 0.3 |
| (3,345) | 1:35:A:LYS:H | 1:22:A:LYS:HG3 | 5 | 0.3 |
| (3,342) | 1:113:A:ARG:HB2 | 1:114:A:ARG:H | 3 | 0.3 |
| (3,296) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB3 | 3 | 0.3 |
| (3,291) | 1:114:A:ARG:H | 1:114:A:ARG:HG2 | 2 | 0.3 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 9 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 1 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 2 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 3 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 4 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 5 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 6 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 7 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 8 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 9 | 0.3 |
| (3,197) | 1:60:A:LYS:HB3 | 1:60:A:LYS:HA | 10 | 0.3 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 3 | 0.3 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 5 | 0.3 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 6 | 0.3 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 8 | 0.3 |
| (3,192) | 1:58:A:LYS:HA | 1:58:A:LYS:HB3 | 10 | 0.3 |
| (3,165) | 1:79:A:VAL:HG11 | 1:88:A:GLU:HA | 5 | 0.3 |
| (3,140) | 1:78:A:LEU:HD22 | 1:88:A:GLU:HG3 | 10 | 0.3 |
| (2,609) | 1:119:A:GLN:HE21 | 1:121:A:GLU:HB2 | 4 | 0.3 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 5 | 0.3 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 9 | 0.3 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG11 | 4 | 0.3 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG12 | 4 | 0.3 |
| (2,304) | 1:105:A:ILE:HB | 1:115:A:VAL:HG13 | 4 | 0.3 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 1 | 0.3 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 1 | 0.3 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 5 | 0.3 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 5 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 7 | 0.3 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 7 | 0.3 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 4 | 0.3 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 4 | 0.3 |
| (1,3714) | 1:84:A:TYR:HD1 | 1:87:A:ASN:HD22 | 8 | 0.3 |
| (1,3714) | 1:84:A:TYR:HD2 | 1:87:A:ASN:HD22 | 8 | 0.3 |
| (1,3631) | 1:23:A:ILE:H | 1:32:A:TYR:HB3 | 2 | 0.3 |
| (1,3592) | 1:95:A:ASN:HA | 1:95:A:ASN:HD22 | 2 | 0.3 |
| (1,3545) | 1:66:A:LEU:H | 1:63:A:GLN:HG2 | 4 | 0.3 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 3 | 0.3 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 3 | 0.3 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 3 | 0.3 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 6 | 0.3 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 6 | 0.3 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 6 | 0.3 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 8 | 0.3 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 9 | 0.3 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 3 | 0.3 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 5 | 0.3 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 5 | 0.3 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 5 | 0.3 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 8 | 0.3 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 6 | 0.3 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 6 | 0.3 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 6 | 0.3 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 10 | 0.3 |
| (1,2735) | 1:85:A:ARG:HB3 | 1:87:A:ASN:H | 1 | 0.3 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 10 | 0.3 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 10 | 0.3 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 8 | 0.3 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 6 | 0.3 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 9 | 0.3 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 5 | 0.3 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 4 | 0.3 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 4 | 0.3 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 4 | 0.3 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 4 | 0.3 |
| (1,2047) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 10 | 0.3 |
| (1,2047) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 10 | 0.3 |
| (1,2047) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 10 | 0.3 |
| (1,2046) | 1:68:A:THR:HG21 | 1:124:A:SER:HB2 | 3 | 0.3 |
| (1,2046) | 1:68:A:THR:HG22 | 1:124:A:SER:HB2 | 3 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2046) | 1:68:A:THR:HG23 | 1:124:A:SER:HB2 | 3 | 0.3 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 9 | 0.3 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 9 | 0.3 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 9 | 0.3 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 1 | 0.3 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 8 | 0.3 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 7 | 0.3 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 8 | 0.3 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 8 | 0.3 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 8 | 0.3 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB1 | 6 | 0.3 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB2 | 6 | 0.3 |
| (1,1214) | 1:73:A:PRO:HD3 | 1:72:A:ALA:HB3 | 6 | 0.3 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG21 | 1 | 0.3 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG22 | 1 | 0.3 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG23 | 1 | 0.3 |
| (1,832) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 5 | 0.3 |
| (1,700) | 1:43:A:ILE:HG12 | 1:41:A:GLU:HG3 | 4 | 0.3 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 7 | 0.3 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 7 | 0.3 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 7 | 0.3 |
| (1,673) | 1:41:A:GLU:HG3 | 1:43:A:ILE:HA | 7 | 0.3 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 1 | 0.3 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 1 | 0.3 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 1 | 0.3 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 6 | 0.3 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG21 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG22 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG11 | 1:39:A:VAL:HG23 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG21 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG22 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG12 | 1:39:A:VAL:HG23 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG21 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG22 | 9 | 0.3 |
| (1,578) | 1:42:A:VAL:HG13 | 1:39:A:VAL:HG23 | 9 | 0.3 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 4 | 0.3 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 4 | 0.3 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 4 | 0.3 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 10 | 0.3 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 10 | 0.3 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 10 | 0.3 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 1 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,25) | 1:7:A:ARG:HA | 1:7:A:ARG:HG2 | 3 | 0.3 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 7 | 0.3 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 8 | 0.3 |
| (1,12) | 1:96:A:GLU:HB2 | 1:96:A:GLU:H | 10 | 0.3 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG22 | 2 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG23 | 5 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 6 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG21 | 7 | 0.29 |
| (3,1184) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 3 | 0.29 |
| (3,1174) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD2 | 1 | 0.29 |
| (3,1170) | 1:111:A:LYS:HB2 | 1:112:A:GLY:H | 5 | 0.29 |
| (3,1128) | 1:72:A:ALA:H | 1:71:A:PRO:HB3 | 5 | 0.29 |
| (3,1128) | 1:75:A:LYS:HG2 | 1:72:A:ALA:H | 8 | 0.29 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 6 | 0.29 |
| (3,1091) | 1:115:A:VAL:H | 1:105:A:ILE:H | 6 | 0.29 |
| (3,995) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 2 | 0.29 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 2 | 0.29 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG23 | 9 | 0.29 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG21 | 8 | 0.29 |
| (3,885) | 1:69:A:VAL:HG21 | 1:69:A:VAL:HB | 3 | 0.29 |
| (3,885) | 1:69:A:VAL:HG22 | 1:69:A:VAL:HB | 8 | 0.29 |
| (3,885) | 1:69:A:VAL:HG22 | 1:69:A:VAL:HB | 10 | 0.29 |
| (3,841) | 1:80:A:LEU:H | 1:123:A:ILE:HG23 | 4 | 0.29 |
| (3,767) | 1:77:A:ILE:H | 1:77:A:ILE:HD13 | 1 | 0.29 |
| (3,743) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HA | 4 | 0.29 |
| (3,743) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HA | 5 | 0.29 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD11 | 3 | 0.29 |
| (3,640) | 1:6:A:LYS:HA | 1:6:A:LYS:H | 7 | 0.29 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD11 | 1 | 0.29 |
| (3,602) | 1:61:A:LEU:HG | 1:61:A:LEU:HD13 | 9 | 0.29 |
| (3,595) | 1:105:A:ILE:HB | 1:106:A:GLU:H | 10 | 0.29 |
| (3,518) | 1:26:A:LYS:HD2 | 1:30:A:GLU:HG2 | 2 | 0.29 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 3 | 0.29 |
| (3,371) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 8 | 0.29 |
| (3,187) | 1:16:A:GLN:H | 1:14:A:TRP:HZ3 | 6 | 0.29 |
| (3,177) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 10 | 0.29 |
| (3,153) | 1:123:A:ILE:HD11 | 1:102:A:THR:H | 5 | 0.29 |
| (3,144) | 1:96:A:GLU:HB3 | 1:97:A:LYS:H | 4 | 0.29 |
| (3,23) | 1:127:A:ALA:HB2 | 1:18:A:GLU:H | 3 | 0.29 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 1 | 0.29 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD21 | 3 | 0.29 |
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD22 | 3 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,398) | 1:13:A:TYR:HB3 | 1:15:A:LEU:HD23 | 3 | 0.29 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 2 | 0.29 |
| (2,222) | 1:75:A:LYS:HA | 1:76:A:ARG:HD2 | 10 | 0.29 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 3 | 0.29 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 4 | 0.29 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 4 | 0.29 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 10 | 0.29 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 7 | 0.29 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 8 | 0.29 |
| (1,3695) | 1:68:A:THR:H | 1:121:A:GLU:HB3 | 9 | 0.29 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 2 | 0.29 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 9 | 0.29 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 3 | 0.29 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 1 | 0.29 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 1 | 0.29 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 1 | 0.29 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 1 | 0.29 |
| (1,3391) | 1:11:A:THR:H | 1:81:A:ASN:HD22 | 1 | 0.29 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 3 | 0.29 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 10 | 0.29 |
| (1,3098) | 1:44:A:ASP:HB2 | 1:47:A:THR:H | 5 | 0.29 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 3 | 0.29 |
| (1,2906) | 1:68:A:THR:H | 1:66:A:LEU:HA | 1 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 6 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 6 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 6 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 7 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 7 | 0.29 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 7 | 0.29 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 7 | 0.29 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 6 | 0.29 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 6 | 0.29 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 6 | 0.29 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 5 | 0.29 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 7 | 0.29 |
| (1,2622) | 1:97:A:LYS:H | 1:97:A:LYS:HG3 | 5 | 0.29 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 7 | 0.29 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 8 | 0.29 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 1 | 0.29 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG11 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG12 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG13 | 8 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG11 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG12 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG13 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG11 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG12 | 8 | 0.29 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG13 | 8 | 0.29 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 2 | 0.29 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 2 | 0.29 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 2 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 6 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 9 | 0.29 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 9 | 0.29 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 4 | 0.29 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 5 | 0.29 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 5 | 0.29 |
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 5 | 0.29 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 7 | 0.29 |
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 7 | 0.29 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 7 | 0.29 |
| (1,2137) | 1:119:A:GLN:HG2 | 1:100:A:SER:HB2 | 5 | 0.29 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 4 | 0.29 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 5 | 0.29 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 4 | 0.29 |
| (1,1898) | 1:115:A:VAL:H | 1:114:A:ARG:HG2 | 4 | 0.29 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 3 | 0.29 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 4 | 0.29 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 4 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 4 | 0.29 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 3 | 0.29 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 3 | 0.29 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 3 | 0.29 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 3 | 0.29 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 3 | 0.29 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 3 | 0.29 |
| (1,1657) | 1:101:A:ALA:HB1 | 1:95:A:ASN:H | 1 | 0.29 |
| (1,1657) | 1:101:A:ALA:HB2 | 1:95:A:ASN:H | 1 | 0.29 |
| (1,1657) | 1:101:A:ALA:HB3 | 1:95:A:ASN:H | 1 | 0.29 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 2 | 0.29 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 7 | 0.29 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 4 | 0.29 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 9 | 0.29 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 9 | 0.29 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 9 | 0.29 |
| (1,1263) | 1:76:A:ARG:HG3 | 1:76:A:ARG:HA | 10 | 0.29 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 8 | 0.29 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD11 | 10 | 0.29 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD12 | 10 | 0.29 |
| (1,856) | 1:38:A:ILE:H | 1:53:A:ILE:HD13 | 10 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 5 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 5 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 5 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 6 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 6 | 0.29 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 6 | 0.29 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG21 | 8 | 0.29 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG22 | 8 | 0.29 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG23 | 8 | 0.29 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 8 | 0.29 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 8 | 0.29 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 8 | 0.29 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 9 | 0.29 |
| (1,621) | 1:41:A:GLU:HA | 1:41:A:GLU:HG3 | 4 | 0.29 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 2 | 0.29 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 2 | 0.29 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 2 | 0.29 |
| (1,588) | 1:53:A:ILE:HA | 1:38:A:ILE:HG12 | 9 | 0.29 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 8 | 0.29 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 8 | 0.29 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 8 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 4 | 0.29 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 4 | 0.29 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 4 | 0.29 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 3 | 0.29 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 3 | 0.29 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 3 | 0.29 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 4 | 0.29 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 4 | 0.29 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 4 | 0.29 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 7 | 0.29 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 7 | 0.29 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 7 | 0.29 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 10 | 0.29 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 10 | 0.29 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 10 | 0.29 |
| (1,29) | 1:7:A:ARG:HD3 | 1:7:A:ARG:HB2 | 7 | 0.29 |
| (1,1) | 1:107:A:THR:HB | 1:108:A:GLY:H | 2 | 0.29 |
| (3,1210) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 1 | 0.28 |
| (3,1210) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG22 | 3 | 0.28 |
| (3,1210) | 1:104:A:VAL:HG11 | 1:104:A:VAL:HG23 | 4 | 0.28 |
| (3,1210) | 1:104:A:VAL:HG12 | 1:104:A:VAL:HG22 | 8 | 0.28 |
| (3,1210) | 1:104:A:VAL:HG13 | 1:104:A:VAL:HG22 | 9 | 0.28 |
| (3,1164) | 1:28:A:LEU:HD21 | 1:29:A:GLY:H | 9 | 0.28 |
| (3,1142) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HG2 | 7 | 0.28 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 3 | 0.28 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 1 | 0.28 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 1 | 0.28 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 4 | 0.28 |
| (3,936) | 1:77:A:ILE:HG13 | 1:103:A:ILE:HB | 10 | 0.28 |
| (3,885) | 1:69:A:VAL:HG22 | 1:69:A:VAL:HB | 6 | 0.28 |
| (3,885) | 1:69:A:VAL:HG22 | 1:69:A:VAL:HB | 7 | 0.28 |
| (3,751) | 1:43:A:ILE:HG22 | 1:43:A:ILE:H | 8 | 0.28 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 8 | 0.28 |
| (3,560) | 1:31:A:LYS:HG3 | 1:33:A:HIS:H | 8 | 0.28 |
| (3,471) | 1:127:A:ALA:HB3 | 1:20:A:ILE:H | 8 | 0.28 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 7 | 0.28 |
| (3,378) | 1:89:A:GLY:H | 1:103:A:ILE:HD12 | 2 | 0.28 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 7 | 0.28 |
| (3,303) | 1:102:A:THR:HA | 1:103:A:ILE:HD11 | 1 | 0.28 |
| (3,296) | 1:91:A:LEU:HD23 | 1:91:A:LEU:HG | 1 | 0.28 |
| (3,280) | 1:112:A:GLY:H | 1:111:A:LYS:HG3 | 6 | 0.28 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD12 | 8 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,626) | 1:48:A:ALA:H | 1:60:A:LYS:HE3 | 10 | 0.28 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 7 | 0.28 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 2 | 0.28 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 2 | 0.28 |
| (1,3753) | 1:34:A:LYS:HD2 | 1:33:A:HIS:HE1 | 8 | 0.28 |
| (1,3726) | 1:95:A:ASN:HD21 | 1:98:A:THR:HB | 7 | 0.28 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 2 | 0.28 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 6 | 0.28 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 4 | 0.28 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 7 | 0.28 |
| (1,3453) | 1:14:A:TRP:HA | 1:16:A:GLN:HE22 | 5 | 0.28 |
| (1,3126) | 1:44:A:ASP:H | 1:47:A:THR:HA | 5 | 0.28 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 4 | 0.28 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 2 | 0.28 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 2 | 0.28 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 2 | 0.28 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 3 | 0.28 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 10 | 0.28 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 10 | 0.28 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 10 | 0.28 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 5 | 0.28 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 4 | 0.28 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 9 | 0.28 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 9 | 0.28 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 9 | 0.28 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 5 | 0.28 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 1 | 0.28 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 1 | 0.28 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 1 | 0.28 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 10 | 0.28 |
| (1,2447) | 1:115:A:VAL:HB | 1:115:A:VAL:H | 2 | 0.28 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 8 | 0.28 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 3 | 0.28 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 1 | 0.28 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 1 | 0.28 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 1 | 0.28 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 1 | 0.28 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB1 | 3 | 0.28 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB2 | 3 | 0.28 |
| (1,2244) | 1:15:A:LEU:HB2 | 1:48:A:ALA:HB3 | 3 | 0.28 |
| (1,2197) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 6 | 0.28 |
| (1,2161) | 1:115:A:VAL:HG21 | 1:118:A:ILE:HG13 | 5 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2161) | 1:115:A:VAL:HG22 | 1:118:A:ILE:HG13 | 5 | 0.28 |
| (1,2161) | 1:115:A:VAL:HG23 | 1:118:A:ILE:HG13 | 5 | 0.28 |
| (1,2095) | 1:127:A:ALA:HB1 | 1:18:A:GLU:HG2 | 4 | 0.28 |
| (1,2095) | 1:127:A:ALA:HB2 | 1:18:A:GLU:HG2 | 4 | 0.28 |
| (1,2095) | 1:127:A:ALA:HB3 | 1:18:A:GLU:HG2 | 4 | 0.28 |
| (1,2071) | 1:126:A:LEU:HB2 | 1:76:A:ARG:HB3 | 7 | 0.28 |
| (1,2007) | 1:78:A:LEU:H | 1:123:A:ILE:HA | 7 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 1 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 3 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 6 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 7 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 8 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 9 | 0.28 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 10 | 0.28 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 5 | 0.28 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 5 | 0.28 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 5 | 0.28 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 6 | 0.28 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 1 | 0.28 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 3 | 0.28 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 9 | 0.28 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 10 | 0.28 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 7 | 0.28 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 7 | 0.28 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 7 | 0.28 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 9 | 0.28 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 6 | 0.28 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 6 | 0.28 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 6 | 0.28 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 6 | 0.28 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG21 | 6 | 0.28 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG22 | 6 | 0.28 |
| (1,1321) | 1:71:A:PRO:HG2 | 1:77:A:ILE:HG23 | 6 | 0.28 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 3 | 0.28 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 3 | 0.28 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 3 | 0.28 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 1 | 0.28 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 7 | 0.28 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 2 | 0.28 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 7 | 0.28 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 10 | 0.28 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG21 | 2 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG22 | 2 | 0.28 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG23 | 2 | 0.28 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 4 | 0.28 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 4 | 0.28 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 4 | 0.28 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 1 | 0.28 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 1 | 0.28 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 1 | 0.28 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 1 | 0.28 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 1 | 0.28 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 1 | 0.28 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 9 | 0.28 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 9 | 0.28 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 9 | 0.28 |
| (1,584) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HD11 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HD12 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HD13 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HD11 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HD12 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HD13 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HD11 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HD12 | 7 | 0.28 |
| (1,584) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HD13 | 7 | 0.28 |
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 3 | 0.28 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 3 | 0.28 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 3 | 0.28 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 4 | 0.28 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 8 | 0.28 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 5 | 0.28 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 5 | 0.28 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 5 | 0.28 |
| (1,169) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HG3 | 5 | 0.28 |
| (1,169) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HG3 | 5 | 0.28 |
| (1,169) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HG3 | 5 | 0.28 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 4 | 0.28 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 4 | 0.28 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 4 | 0.28 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 5 | 0.28 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 5 | 0.28 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 5 | 0.28 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 7 | 0.28 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 7 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 7 | 0.28 |
| (3,1174) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD2 | 7 | 0.27 |
| (3,1173) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HG2 | 3 | 0.27 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 7 | 0.27 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 1 | 0.27 |
| (3,1155) | 1:118:A:ILE:HG22 | 1:119:A:GLN:H | 6 | 0.27 |
| (3,1154) | 1:6:A:LYS:HB3 | 1:7:A:ARG:H | 4 | 0.27 |
| (3,1087) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HB3 | 8 | 0.27 |
| (3,1087) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HB3 | 8 | 0.27 |
| (3,1087) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HB3 | 8 | 0.27 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 5 | 0.27 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 7 | 0.27 |
| (3,928) | 1:94:A:ILE:HG23 | 1:91:A:LEU:HA | 5 | 0.27 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 3 | 0.27 |
| (3,751) | 1:43:A:ILE:HG22 | 1:43:A:ILE:H | 3 | 0.27 |
| (3,743) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HA | 8 | 0.27 |
| (3,676) | 1:108:A:GLY:H | 1:107:A:THR:HG23 | 4 | 0.27 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 10 | 0.27 |
| (3,555) | 1:12:A:ASP:HB2 | 1:46:A:TYR:HE2 | 3 | 0.27 |
| (3,441) | 1:23:A:ILE:H | 1:22:A:LYS:HG3 | 5 | 0.27 |
| (3,423) | 1:61:A:LEU:HD13 | 1:25:A:THR:H | 4 | 0.27 |
| (3,423) | 1:61:A:LEU:HD12 | 1:25:A:THR:H | 9 | 0.27 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD12 | 1 | 0.27 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 1 | 0.27 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 2 | 0.27 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 7 | 0.27 |
| (3,109) | 1:4:A:GLU:HB2 | 1:4:A:GLU:HG3 | 10 | 0.27 |
| (3,21) | 1:126:A:LEU:HD22 | 1:88:A:GLU:HG2 | 4 | 0.27 |
| (2,626) | 1:48:A:ALA:H | 1:60:A:LYS:HE3 | 5 | 0.27 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 1 | 0.27 |
| (2,520) | 1:78:A:LEU:H | 1:88:A:GLU:HG2 | 1 | 0.27 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 7 | 0.27 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 7 | 0.27 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 7 | 0.27 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 6 | 0.27 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 6 | 0.27 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 3 | 0.27 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 3 | 0.27 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 7 | 0.27 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 7 | 0.27 |
| (1,3714) | 1:84:A:TYR:HD1 | 1:87:A:ASN:HD22 | 10 | 0.27 |
| (1,3714) | 1:84:A:TYR:HD2 | 1:87:A:ASN:HD22 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 10 | 0.27 |
| (1,3499) | 1:37:A:ALA:H | 1:36:A:LYS:HE2 | 1 | 0.27 |
| (1,3412) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 5 | 0.27 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 6 | 0.27 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 5 | 0.27 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 7 | 0.27 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 8 | 0.27 |
| (1,3000) | 1:59:A:LEU:HD11 | 1:60:A:LYS:H | 4 | 0.27 |
| (1,3000) | 1:59:A:LEU:HD12 | 1:60:A:LYS:H | 4 | 0.27 |
| (1,3000) | 1:59:A:LEU:HD13 | 1:60:A:LYS:H | 4 | 0.27 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 9 | 0.27 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 9 | 0.27 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 9 | 0.27 |
| (1,2841) | 1:111:A:LYS:HE3 | 1:112:A:GLY:H | 3 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 1 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 1 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 1 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 8 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 8 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 8 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 9 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 9 | 0.27 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 9 | 0.27 |
| (1,2794) | 1:81:A:ASN:H | 1:80:A:LEU:HB3 | 1 | 0.27 |
| (1,2781) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 2 | 0.27 |
| (1,2765) | 1:104:A:VAL:HA | 1:90:A:THR:H | 3 | 0.27 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 3 | 0.27 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 6 | 0.27 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 6 | 0.27 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 6 | 0.27 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 4 | 0.27 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 9 | 0.27 |
| (1,2633) | 1:96:A:GLU:H | 1:95:A:ASN:HB3 | 1 | 0.27 |
| (1,2633) | 1:96:A:GLU:H | 1:95:A:ASN:HB3 | 2 | 0.27 |
| (1,2494) | 1:108:A:GLY:H | 1:111:A:LYS:HE3 | 3 | 0.27 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 8 | 0.27 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 3 | 0.27 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 1 | 0.27 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 7 | 0.27 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 7 | 0.27 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 9 | 0.27 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 9 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 9 | 0.27 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD3 | 4 | 0.27 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 2 | 0.27 |
| (1,2205) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 10 | 0.27 |
| (1,2205) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 10 | 0.27 |
| (1,2205) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 10 | 0.27 |
| (1,2171) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HD11 | 6 | 0.27 |
| (1,2171) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HD12 | 6 | 0.27 |
| (1,2171) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HD13 | 6 | 0.27 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 7 | 0.27 |
| (1,1970) | 1:119:A:GLN:HA | 1:119:A:GLN:HB2 | 2 | 0.27 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 7 | 0.27 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 1 | 0.27 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 5 | 0.27 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 5 | 0.27 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 5 | 0.27 |
| (1,1655) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 3 | 0.27 |
| (1,1655) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 3 | 0.27 |
| (1,1655) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 3 | 0.27 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 4 | 0.27 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 6 | 0.27 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 2 | 0.27 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 2 | 0.27 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 2 | 0.27 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 4 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 7 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 7 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 7 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 10 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 10 | 0.27 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 10 | 0.27 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 3 | 0.27 |
| (1,1256) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA3 | 3 | 0.27 |
| (1,1256) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA3 | 3 | 0.27 |
| (1,1256) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA3 | 3 | 0.27 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 9 | 0.27 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 9 | 0.27 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 9 | 0.27 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 3 | 0.27 |
| (1,832) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 6 | 0.27 |
| (1,817) | 1:51:A:LYS:HG2 | 1:56:A:GLY:HA3 | 8 | 0.27 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 10 | 0.27 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 10 | 0.27 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 10 | 0.27 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 10 | 0.27 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 10 | 0.27 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 5 | 0.27 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 9 | 0.27 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 9 | 0.27 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 9 | 0.27 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 4 | 0.27 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 4 | 0.27 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 4 | 0.27 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 4 | 0.27 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 6 | 0.27 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 6 | 0.27 |
| (1,565) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 6 | 0.27 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 5 | 0.27 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 5 | 0.27 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 5 | 0.27 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 6 | 0.27 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 6 | 0.27 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 6 | 0.27 |
| (3,1174) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD2 | 9 | 0.26 |
| (3,1157) | 1:80:A:LEU:HD13 | 1:14:A:TRP:HZ3 | 2 | 0.26 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 8 | 0.26 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 2 | 0.26 |
| (3,993) | 1:58:A:LYS:HG3 | 1:50:A:VAL:H | 5 | 0.26 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 9 | 0.26 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG23 | 3 | 0.26 |
| (3,838) | 1:53:A:ILE:H | 1:52:A:MET:H | 3 | 0.26 |
| (3,838) | 1:52:A:MET:H | 1:59:A:LEU:H | 10 | 0.26 |
| (3,820) | 1:117:A:GLY:H | 1:116:A:GLU:HG2 | 6 | 0.26 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 10 | 0.26 |
| (3,735) | 1:115:A:VAL:HG13 | 1:103:A:ILE:HD11 | 5 | 0.26 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 10 | 0.26 |
| (3,640) | 1:4:A:GLU:HA | 1:5:A:LYS:H | 9 | 0.26 |
| (3,600) | 1:20:A:ILE:HB | 1:21:A:VAL:H | 8 | 0.26 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD11 | 5 | 0.26 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD13 | 10 | 0.26 |
| (3,537) | 1:76:A:ARG:H | 1:76:A:ARG:HD2 | 7 | 0.26 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 10 | 0.26 |
| (3,399) | 1:45:A:LYS:HG3 | 1:44:A:ASP:HA | 4 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,303) | 1:102:A:THR:HA | 1:103:A:ILE:HD11 | 7 | 0.26 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 3 | 0.26 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 9 | 0.26 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 10 | 0.26 |
| (3,153) | 1:91:A:LEU:HD11 | 1:102:A:THR:H | 7 | 0.26 |
| (3,129) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HB | 9 | 0.26 |
| (3,128) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 3 | 0.26 |
| (3,109) | 1:4:A:GLU:HB3 | 1:4:A:GLU:HG3 | 3 | 0.26 |
| (3,109) | 1:3:A:GLU:HB2 | 1:3:A:GLU:HG3 | 5 | 0.26 |
| (3,109) | 1:4:A:GLU:HB3 | 1:4:A:GLU:HG2 | 8 | 0.26 |
| (2,617) | 1:24:A:ILE:HA | 1:33:A:HIS:H | 6 | 0.26 |
| (2,591) | 1:11:A:THR:H | 1:13:A:TYR:HD1 | 3 | 0.26 |
| (2,591) | 1:11:A:THR:H | 1:13:A:TYR:HD2 | 3 | 0.26 |
| (2,589) | 1:82:A:GLY:HA3 | 1:11:A:THR:H | 9 | 0.26 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 1 | 0.26 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 8 | 0.26 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 8 | 0.26 |
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 8 | 0.26 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 8 | 0.26 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 3 | 0.26 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 7 | 0.26 |
| (1,3592) | 1:95:A:ASN:HA | 1:95:A:ASN:HD22 | 1 | 0.26 |
| (1,3591) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD21 | 3 | 0.26 |
| (1,3591) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD21 | 3 | 0.26 |
| (1,3591) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD21 | 3 | 0.26 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG21 | 1 | 0.26 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG22 | 1 | 0.26 |
| (1,3422) | 1:10:A:ARG:H | 1:11:A:THR:HG23 | 1 | 0.26 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 9 | 0.26 |
| (1,3391) | 1:11:A:THR:H | 1:81:A:ASN:HD22 | 5 | 0.26 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 1 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 4 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 4 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 4 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 8 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 8 | 0.26 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 8 | 0.26 |
| (1,3133) | 1:44:A:ASP:H | 1:43:A:ILE:HG12 | 8 | 0.26 |
| (1,2985) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 3 | 0.26 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 5 | 0.26 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 7 | 0.26 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 3 | 0.26 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 3 | 0.26 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 2 | 0.26 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 3 | 0.26 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 2 | 0.26 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 9 | 0.26 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 5 | 0.26 |
| (1,2447) | 1:115:A:VAL:HB | 1:115:A:VAL:H | 7 | 0.26 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 2 | 0.26 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 9 | 0.26 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 3 | 0.26 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 2 | 0.26 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 4 | 0.26 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 4 | 0.26 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 4 | 0.26 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 5 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 3 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 8 | 0.26 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 8 | 0.26 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 2 | 0.26 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 2 | 0.26 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 2 | 0.26 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 2 | 0.26 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 2 | 0.26 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 2 | 0.26 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 9 | 0.26 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 9 | 0.26 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG21 | 10 | 0.26 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG22 | 10 | 0.26 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG23 | 10 | 0.26 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 7 | 0.26 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 8 | 0.26 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 1 | 0.26 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 1 | 0.26 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 1 | 0.26 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 8 | 0.26 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 8 | 0.26 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 8 | 0.26 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 2 | 0.26 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 4 | 0.26 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 10 | 0.26 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 9 | 0.26 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 2 | 0.26 |
| (1,1434) | 1:85:A:ARG:HA | 1:81:A:ASN:HA | 1 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 1 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 1 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 1 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 2 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 2 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 2 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 3 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 3 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 3 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 4 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 4 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 4 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 5 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 5 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 5 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 6 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 6 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 6 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 8 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 8 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 8 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG11 | 1:79:A:VAL:HA | 9 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG12 | 1:79:A:VAL:HA | 9 | 0.26 |
| (1,1338) | 1:79:A:VAL:HG13 | 1:79:A:VAL:HA | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 5 | 0.26 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 6 | 0.26 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 9 | 0.26 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 7 | 0.26 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 7 | 0.26 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 7 | 0.26 |
| (1,816) | 1:111:A:LYS:HD3 | 1:106:A:GLU:HA | 6 | 0.26 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 9 | 0.26 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 9 | 0.26 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 9 | 0.26 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG21 | 1 | 0.26 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG22 | 1 | 0.26 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG23 | 1 | 0.26 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 1 | 0.26 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 4 | 0.26 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 9 | 0.26 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 10 | 0.26 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 7 | 0.26 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 7 | 0.26 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 7 | 0.26 |
| (1,423) | 1:26:A:LYS:HG3 | 1:26:A:LYS:HE2 | 2 | 0.26 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 1 | 0.26 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 1 | 0.26 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 1 | 0.26 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 7 | 0.26 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 7 | 0.26 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 7 | 0.26 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 2 | 0.26 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 2 | 0.26 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 2 | 0.26 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 2 | 0.26 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 2 | 0.26 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 2 | 0.26 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 3 | 0.26 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 3 | 0.26 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 3 | 0.26 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 1 | 0.26 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 1 | 0.26 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 1 | 0.26 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 8 | 0.26 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 8 | 0.26 |
| (1,138) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 8 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 10 | 0.26 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 10 | 0.26 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 10 | 0.26 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 3 | 0.26 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 3 | 0.26 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 3 | 0.26 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 6 | 0.26 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 6 | 0.26 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 6 | 0.26 |
| (1,42) | 1:8:A:THR:HA | 1:9:A:ALA:H | 1 | 0.26 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 7 | 0.26 |
| (3,1226) | 1:117:A:GLY:H | 1:116:A:GLU:HG2 | 6 | 0.25 |
| (3,1170) | 1:111:A:LYS:HB2 | 1:112:A:GLY:H | 8 | 0.25 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 4 | 0.25 |
| (3,1137) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 3 | 0.25 |
| (3,1091) | 1:112:A:GLY:H | 1:105:A:ILE:H | 7 | 0.25 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 3 | 0.25 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD13 | 3 | 0.25 |
| (3,863) | 1:113:A:ARG:HD3 | 1:103:A:ILE:HD13 | 5 | 0.25 |
| (3,721) | 1:51:A:LYS:HG3 | 1:57:A:ASP:HA | 1 | 0.25 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD12 | 3 | 0.25 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD11 | 9 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 1 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 2 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 3 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 5 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 6 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 7 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 8 | 0.25 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 9 | 0.25 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 5 | 0.25 |
| (3,634) | 1:103:A:ILE:HG12 | 1:104:A:VAL:H | 6 | 0.25 |
| (3,613) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 3 | 0.25 |
| (3,613) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 5 | 0.25 |
| (3,613) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 7 | 0.25 |
| (3,613) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 8 | 0.25 |
| (3,613) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HB3 | 10 | 0.25 |
| (3,595) | 1:105:A:ILE:HB | 1:106:A:GLU:H | 2 | 0.25 |
| (3,545) | 1:49:A:VAL:HG12 | 1:49:A:VAL:HA | 3 | 0.25 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 3 | 0.25 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 2 | 0.25 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 6 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,423) | 1:61:A:LEU:HD13 | 1:25:A:THR:H | 5 | 0.25 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 1 | 0.25 |
| (3,396) | 1:118:A:ILE:HG23 | 1:121:A:GLU:HA | 1 | 0.25 |
| (3,297) | 1:42:A:VAL:HG12 | 1:16:A:GLN:HG3 | 5 | 0.25 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD13 | 9 | 0.25 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 4 | 0.25 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 6 | 0.25 |
| (3,85) | 1:39:A:VAL:HG21 | 1:50:A:VAL:HA | 6 | 0.25 |
| (2,574) | 1:39:A:VAL:H | 1:20:A:ILE:HG12 | 1 | 0.25 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 8 | 0.25 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 6 | 0.25 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 6 | 0.25 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 8 | 0.25 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 8 | 0.25 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 5 | 0.25 |
| (1,3635) | 1:64:A:THR:H | 1:62:A:ASP:H | 1 | 0.25 |
| (1,3606) | 1:119:A:GLN:HE22 | 1:100:A:SER:HB2 | 6 | 0.25 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 8 | 0.25 |
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 8 | 0.25 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 8 | 0.25 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 2 | 0.25 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 7 | 0.25 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG21 | 4 | 0.25 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG22 | 4 | 0.25 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG23 | 4 | 0.25 |
| (1,3097) | 1:46:A:TYR:HB3 | 1:47:A:THR:H | 1 | 0.25 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 9 | 0.25 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 4 | 0.25 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 1 | 0.25 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 1 | 0.25 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 1 | 0.25 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG21 | 3 | 0.25 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG22 | 3 | 0.25 |
| (1,2888) | 1:70:A:ILE:H | 1:69:A:VAL:HG23 | 3 | 0.25 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 10 | 0.25 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 2 | 0.25 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 2 | 0.25 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 2 | 0.25 |
| (1,2749) | 1:85:A:ARG:HG3 | 1:86:A:GLY:H | 2 | 0.25 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 1 | 0.25 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 3 | 0.25 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 3 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 3 | 0.25 |
| (1,2622) | 1:97:A:LYS:H | 1:97:A:LYS:HG3 | 8 | 0.25 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 2 | 0.25 |
| (1,2608) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 9 | 0.25 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 10 | 0.25 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 4 | 0.25 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 4 | 0.25 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 4 | 0.25 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 7 | 0.25 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 2 | 0.25 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 3 | 0.25 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 5 | 0.25 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 1 | 0.25 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 3 | 0.25 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 5 | 0.25 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 7 | 0.25 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 9 | 0.25 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 10 | 0.25 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 3 | 0.25 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 5 | 0.25 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 5 | 0.25 |
| (1,2271) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HA | 3 | 0.25 |
| (1,2271) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HA | 3 | 0.25 |
| (1,2271) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HA | 3 | 0.25 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG21 | 9 | 0.25 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 9 | 0.25 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG23 | 9 | 0.25 |
| (1,2238) | 1:76:A:ARG:HD2 | 1:90:A:THR:HA | 9 | 0.25 |
| (1,2166) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HG2 | 8 | 0.25 |
| (1,2166) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HG2 | 8 | 0.25 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 5 | 0.25 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 7 | 0.25 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 7 | 0.25 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 7 | 0.25 |
| (1,2123) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HD11 | 9 | 0.25 |
| (1,2123) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HD12 | 9 | 0.25 |
| (1,2123) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HD13 | 9 | 0.25 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 7 | 0.25 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 7 | 0.25 |
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 7 | 0.25 |
| (1,1971) | 1:119:A:GLN:HA | 1:101:A:ALA:H | 6 | 0.25 |
| (1,1966) | 1:118:A:ILE:HG21 | 1:122:A:ASP:H | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1966) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 2 | 0.25 |
| (1,1966) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 2 | 0.25 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 9 | 0.25 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 4 | 0.25 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 4 | 0.25 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 2 | 0.25 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 2 | 0.25 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 2 | 0.25 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 6 | 0.25 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG21 | 2 | 0.25 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG22 | 2 | 0.25 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG23 | 2 | 0.25 |
| (1,1682) | 1:47:A:THR:HG21 | 1:43:A:ILE:HB | 8 | 0.25 |
| (1,1682) | 1:47:A:THR:HG22 | 1:43:A:ILE:HB | 8 | 0.25 |
| (1,1682) | 1:47:A:THR:HG23 | 1:43:A:ILE:HB | 8 | 0.25 |
| (1,1648) | 1:101:A:ALA:H | 1:100:A:SER:HB3 | 3 | 0.25 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 8 | 0.25 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 3 | 0.25 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 1 | 0.25 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 1 | 0.25 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 1 | 0.25 |
| (1,1352) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA2 | 4 | 0.25 |
| (1,1352) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA2 | 4 | 0.25 |
| (1,1352) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA2 | 4 | 0.25 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 1 | 0.25 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 1 | 0.25 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 1 | 0.25 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 10 | 0.25 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 10 | 0.25 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 10 | 0.25 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 5 | 0.25 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 10 | 0.25 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 4 | 0.25 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 1 | 0.25 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 4 | 0.25 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 5 | 0.25 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 8 | 0.25 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 10 | 0.25 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 10 | 0.25 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 10 | 0.25 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 10 | 0.25 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD21 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD22 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG21 | 1:59:A:LEU:HD23 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD21 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD22 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG22 | 1:59:A:LEU:HD23 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD21 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD22 | 4 | 0.25 |
| (1,804) | 1:50:A:VAL:HG23 | 1:59:A:LEU:HD23 | 4 | 0.25 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 4 | 0.25 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 4 | 0.25 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 4 | 0.25 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 2 | 0.25 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 2 | 0.25 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 2 | 0.25 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 10 | 0.25 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 10 | 0.25 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 10 | 0.25 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 2 | 0.25 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 6 | 0.25 |
| (1,693) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 1 | 0.25 |
| (1,693) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 1 | 0.25 |
| (1,693) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 1 | 0.25 |
| (1,693) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 6 | 0.25 |
| (1,693) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 6 | 0.25 |
| (1,693) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 6 | 0.25 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 10 | 0.25 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 10 | 0.25 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 10 | 0.25 |
| (1,423) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HE3 | 10 | 0.25 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 3 | 0.25 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 3 | 0.25 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 3 | 0.25 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 4 | 0.25 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 4 | 0.25 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 4 | 0.25 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 7 | 0.25 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 7 | 0.25 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 7 | 0.25 |
| (1,248) | 1:19:A:ILE:HD11 | 1:14:A:TRP:HZ3 | 10 | 0.25 |
| (1,248) | 1:19:A:ILE:HD12 | 1:14:A:TRP:HZ3 | 10 | 0.25 |
| (1,248) | 1:19:A:ILE:HD13 | 1:14:A:TRP:HZ3 | 10 | 0.25 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 2 | 0.25 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 2 | 0.25 |
| (1,25) | 1:7:A:ARG:HA | 1:7:A:ARG:HG2 | 7 | 0.25 |
| (3,1095) | 1:26:A:LYS:HB3 | 1:25:A:THR:H | 10 | 0.24 |
| (3,1076) | 1:5:A:LYS:H | 1:5:A:LYS:HD3 | 1 | 0.24 |
| (3,1030) | 1:53:A:ILE:H | 1:37:A:ALA:H | 5 | 0.24 |
| (3,975) | 1:97:A:LYS:HB2 | 1:98:A:THR:HG22 | 3 | 0.24 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 8 | 0.24 |
| (3,951) | 1:124:A:SER:H | 1:123:A:ILE:HG23 | 1 | 0.24 |
| (3,885) | 1:69:A:VAL:HG22 | 1:125:A:LYS:HB2 | 9 | 0.24 |
| (3,854) | 1:104:A:VAL:HA | 1:103:A:ILE:HB | 1 | 0.24 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 2 | 0.24 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 5 | 0.24 |
| (3,662) | 1:120:A:TYR:HA | 1:120:A:TYR:HB2 | 4 | 0.24 |
| (3,595) | 1:106:A:GLU:HG3 | 1:106:A:GLU:H | 5 | 0.24 |
| (3,440) | 1:103:A:ILE:H | 1:117:A:GLY:H | 7 | 0.24 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 2 | 0.24 |
| (3,416) | 1:5:A:LYS:H | 1:4:A:GLU:HG3 | 1 | 0.24 |
| (3,296) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB3 | 8 | 0.24 |
| (3,282) | 1:105:A:ILE:H | 1:111:A:LYS:HA | 6 | 0.24 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 8 | 0.24 |
| (3,153) | 1:123:A:ILE:HD11 | 1:102:A:THR:H | 6 | 0.24 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG22 | 7 | 0.24 |
| (3,109) | 1:4:A:GLU:HB3 | 1:4:A:GLU:HG2 | 2 | 0.24 |
| (3,109) | 1:2:A:GLU:HB3 | 1:2:A:GLU:HG2 | 6 | 0.24 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 2 | 0.24 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 3 | 0.24 |
| (3,85) | 1:39:A:VAL:HG21 | 1:50:A:VAL:HA | 1 | 0.24 |
| (2,617) | 1:24:A:ILE:HA | 1:33:A:HIS:H | 10 | 0.24 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 6 | 0.24 |
| (2,574) | 1:39:A:VAL:H | 1:20:A:ILE:HG12 | 5 | 0.24 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 4 | 0.24 |
| (2,142) | 1:10:A:ARG:HA | 1:82:A:GLY:HA3 | 9 | 0.24 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 5 | 0.24 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 5 | 0.24 |
| (1,3840) | 1:46:A:TYR:HE1 | 1:13:A:TYR:HB2 | 9 | 0.24 |
| (1,3840) | 1:46:A:TYR:HE2 | 1:13:A:TYR:HB2 | 9 | 0.24 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 8 | 0.24 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 3 | 0.24 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 7 | 0.24 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 2 | 0.24 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 8 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2873) | 1:91:A:LEU:HD11 | 1:74:A:GLY:H | 10 | 0.24 |
| (1,2873) | 1:91:A:LEU:HD12 | 1:74:A:GLY:H | 10 | 0.24 |
| (1,2873) | 1:91:A:LEU:HD13 | 1:74:A:GLY:H | 10 | 0.24 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 4 | 0.24 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 4 | 0.24 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 4 | 0.24 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 7 | 0.24 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 3 | 0.24 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 3 | 0.24 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 3 | 0.24 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 2 | 0.24 |
| (1,2493) | 1:110:A:LEU:H | 1:110:A:LEU:HD11 | 10 | 0.24 |
| (1,2493) | 1:110:A:LEU:H | 1:110:A:LEU:HD12 | 10 | 0.24 |
| (1,2493) | 1:110:A:LEU:H | 1:110:A:LEU:HD13 | 10 | 0.24 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 4 | 0.24 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 8 | 0.24 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 8 | 0.24 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 8 | 0.24 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 9 | 0.24 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 9 | 0.24 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 9 | 0.24 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 8 | 0.24 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 6 | 0.24 |
| (1,2418) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 1 | 0.24 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 4 | 0.24 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 4 | 0.24 |
| (1,2246) | 1:13:A:TYR:HB3 | 1:45:A:LYS:HD3 | 9 | 0.24 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 6 | 0.24 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 6 | 0.24 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 6 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 4 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 4 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 4 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 4 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 4 | 0.24 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 4 | 0.24 |
| (1,2196) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 6 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 2 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 2 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 2 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 10 | 0.24 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 10 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 10 | 0.24 |
| (1,1997) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 4 | 0.24 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 5 | 0.24 |
| (1,1629) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 5 | 0.24 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 5 | 0.24 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 5 | 0.24 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 5 | 0.24 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 2 | 0.24 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 7 | 0.24 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 8 | 0.24 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 9 | 0.24 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 8 | 0.24 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 3 | 0.24 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 6 | 0.24 |
| (1,1264) | 1:75:A:LYS:HD3 | 1:72:A:ALA:H | 10 | 0.24 |
| (1,1176) | 1:70:A:ILE:H | 1:70:A:ILE:HG13 | 4 | 0.24 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 6 | 0.24 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 6 | 0.24 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 6 | 0.24 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 3 | 0.24 |
| (1,1021) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 6 | 0.24 |
| (1,1021) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 6 | 0.24 |
| (1,1021) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 6 | 0.24 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 3 | 0.24 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 10 | 0.24 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 3 | 0.24 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 2 | 0.24 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 6 | 0.24 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 9 | 0.24 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 10 | 0.24 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG21 | 2 | 0.24 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG22 | 2 | 0.24 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG23 | 2 | 0.24 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 7 | 0.24 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 7 | 0.24 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 7 | 0.24 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 7 | 0.24 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 7 | 0.24 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 7 | 0.24 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 10 | 0.24 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 7 | 0.24 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 7 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 7 | 0.24 |
| (1,530) | 1:37:A:ALA:HB1 | 1:38:A:ILE:H | 5 | 0.24 |
| (1,530) | 1:37:A:ALA:HB2 | 1:38:A:ILE:H | 5 | 0.24 |
| (1,530) | 1:37:A:ALA:HB3 | 1:38:A:ILE:H | 5 | 0.24 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 9 | 0.24 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 9 | 0.24 |
| (1,451) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 9 | 0.24 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 2 | 0.24 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 2 | 0.24 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 2 | 0.24 |
| (3,1182) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 2 | 0.23 |
| (3,1170) | 1:111:A:LYS:HB2 | 1:112:A:GLY:H | 1 | 0.23 |
| (3,1142) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HG2 | 8 | 0.23 |
| (3,1137) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 2 | 0.23 |
| (3,1128) | 1:75:A:LYS:HG2 | 1:72:A:ALA:H | 4 | 0.23 |
| (3,1128) | 1:72:A:ALA:H | 1:71:A:PRO:HB3 | 6 | 0.23 |
| (3,1108) | 1:10:A:ARG:HB3 | 1:81:A:ASN:HD21 | 4 | 0.23 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 5 | 0.23 |
| (3,1091) | 1:112:A:GLY:H | 1:105:A:ILE:H | 2 | 0.23 |
| (3,1076) | 1:5:A:LYS:H | 1:5:A:LYS:HD3 | 4 | 0.23 |
| (3,1030) | 1:36:A:LYS:H | 1:37:A:ALA:H | 4 | 0.23 |
| (3,993) | 1:61:A:LEU:HG | 1:50:A:VAL:H | 9 | 0.23 |
| (3,864) | 1:53:A:ILE:HG22 | 1:53:A:ILE:HB | 2 | 0.23 |
| (3,864) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 8 | 0.23 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 6 | 0.23 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 7 | 0.23 |
| (3,758) | 1:45:A:LYS:HB2 | 1:45:A:LYS:HD3 | 2 | 0.23 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD11 | 8 | 0.23 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 4 | 0.23 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 4 | 0.23 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 8 | 0.23 |
| (3,489) | 1:82:A:GLY:HA3 | 1:81:A:ASN:HB3 | 5 | 0.23 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 3 | 0.23 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 10 | 0.23 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 1 | 0.23 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 5 | 0.23 |
| (3,366) | 1:42:A:VAL:HG21 | 1:16:A:GLN:HG2 | 1 | 0.23 |
| (3,366) | 1:42:A:VAL:HG22 | 1:16:A:GLN:HG2 | 7 | 0.23 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD13 | 3 | 0.23 |
| (3,223) | 1:99:A:PHE:H | 1:99:A:PHE:HB3 | 5 | 0.23 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 4 | 0.23 |
| (3,180) | 1:65:A:HIS:H | 1:62:A:ASP:HB3 | 5 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG22 | 2 | 0.23 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG23 | 3 | 0.23 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG21 | 4 | 0.23 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG23 | 6 | 0.23 |
| (3,109) | 1:3:A:GLU:HB2 | 1:3:A:GLU:HG3 | 4 | 0.23 |
| (3,109) | 1:2:A:GLU:HB3 | 1:2:A:GLU:HG2 | 7 | 0.23 |
| (3,109) | 1:3:A:GLU:HB2 | 1:3:A:GLU:HG3 | 9 | 0.23 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 4 | 0.23 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 5 | 0.23 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 10 | 0.23 |
| (3,85) | 1:36:A:LYS:HA | 1:69:A:VAL:HG11 | 5 | 0.23 |
| (3,4) | 1:102:A:THR:HG22 | 1:116:A:GLU:H | 5 | 0.23 |
| (3,4) | 1:102:A:THR:HG21 | 1:116:A:GLU:H | 9 | 0.23 |
| (2,609) | 1:119:A:GLN:HE21 | 1:121:A:GLU:HB2 | 7 | 0.23 |
| (2,515) | 1:85:A:ARG:HD2 | 1:81:A:ASN:H | 7 | 0.23 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 1 | 0.23 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 7 | 0.23 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 7 | 0.23 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 2 | 0.23 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 2 | 0.23 |
| (1,3759) | 1:27:A:LYS:HG3 | 1:65:A:HIS:HE1 | 10 | 0.23 |
| (1,3753) | 1:34:A:LYS:HD2 | 1:33:A:HIS:HE1 | 3 | 0.23 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 3 | 0.23 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 10 | 0.23 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 2 | 0.23 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 7 | 0.23 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 8 | 0.23 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 5 | 0.23 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 8 | 0.23 |
| (1,3468) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HE21 | 2 | 0.23 |
| (1,3468) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HE21 | 2 | 0.23 |
| (1,3468) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HE21 | 2 | 0.23 |
| (1,3392) | 1:11:A:THR:H | 1:13:A:TYR:H | 4 | 0.23 |
| (1,3389) | 1:82:A:GLY:H | 1:11:A:THR:H | 3 | 0.23 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 4 | 0.23 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 5 | 0.23 |
| (1,3349) | 1:14:A:TRP:HE3 | 1:16:A:GLN:H | 10 | 0.23 |
| (1,3202) | 1:52:A:MET:HA | 1:37:A:ALA:H | 4 | 0.23 |
| (1,3134) | 1:44:A:ASP:H | 1:43:A:ILE:HG13 | 8 | 0.23 |
| (1,3128) | 1:47:A:THR:HB | 1:44:A:ASP:H | 2 | 0.23 |
| (1,3126) | 1:44:A:ASP:H | 1:47:A:THR:HA | 2 | 0.23 |
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 1 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3077) | 1:49:A:VAL:H | 1:43:A:ILE:H | 10 | 0.23 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 4 | 0.23 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 4 | 0.23 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 4 | 0.23 |
| (1,3000) | 1:59:A:LEU:HD11 | 1:60:A:LYS:H | 2 | 0.23 |
| (1,3000) | 1:59:A:LEU:HD12 | 1:60:A:LYS:H | 2 | 0.23 |
| (1,3000) | 1:59:A:LEU:HD13 | 1:60:A:LYS:H | 2 | 0.23 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 9 | 0.23 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 1 | 0.23 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 3 | 0.23 |
| (1,2807) | 1:79:A:VAL:HG11 | 1:80:A:LEU:H | 5 | 0.23 |
| (1,2807) | 1:79:A:VAL:HG12 | 1:80:A:LEU:H | 5 | 0.23 |
| (1,2807) | 1:79:A:VAL:HG13 | 1:80:A:LEU:H | 5 | 0.23 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 4 | 0.23 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 6 | 0.23 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 5 | 0.23 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 2 | 0.23 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 7 | 0.23 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 7 | 0.23 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 7 | 0.23 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 1 | 0.23 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 10 | 0.23 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 7 | 0.23 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 6 | 0.23 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 9 | 0.23 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 3 | 0.23 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 8 | 0.23 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 7 | 0.23 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 10 | 0.23 |
| (1,2339) | 1:77:A:ILE:HA | 1:124:A:SER:H | 9 | 0.23 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 10 | 0.23 |
| (1,2325) | 1:126:A:LEU:H | 1:77:A:ILE:HG21 | 10 | 0.23 |
| (1,2325) | 1:126:A:LEU:H | 1:77:A:ILE:HG22 | 10 | 0.23 |
| (1,2325) | 1:126:A:LEU:H | 1:77:A:ILE:HG23 | 10 | 0.23 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 9 | 0.23 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 9 | 0.23 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 9 | 0.23 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 5 | 0.23 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 5 | 0.23 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 5 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HD11 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HD12 | 7 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2093) | 1:127:A:ALA:HB1 | 1:38:A:ILE:HD13 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HD11 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HD12 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB2 | 1:38:A:ILE:HD13 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HD11 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HD12 | 7 | 0.23 |
| (1,2093) | 1:127:A:ALA:HB3 | 1:38:A:ILE:HD13 | 7 | 0.23 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 4 | 0.23 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 4 | 0.23 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 4 | 0.23 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 8 | 0.23 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 10 | 0.23 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 10 | 0.23 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 10 | 0.23 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 1 | 0.23 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 1 | 0.23 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 1 | 0.23 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 1 | 0.23 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 4 | 0.23 |
| (1,1616) | 1:98:A:THR:HG21 | 1:98:A:THR:H | 3 | 0.23 |
| (1,1616) | 1:98:A:THR:HG22 | 1:98:A:THR:H | 3 | 0.23 |
| (1,1616) | 1:98:A:THR:HG23 | 1:98:A:THR:H | 3 | 0.23 |
| (1,1616) | 1:98:A:THR:HG21 | 1:98:A:THR:H | 9 | 0.23 |
| (1,1616) | 1:98:A:THR:HG22 | 1:98:A:THR:H | 9 | 0.23 |
| (1,1616) | 1:98:A:THR:HG23 | 1:98:A:THR:H | 9 | 0.23 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG21 | 10 | 0.23 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG22 | 10 | 0.23 |
| (1,1584) | 1:120:A:TYR:HD1 | 1:94:A:ILE:HG23 | 10 | 0.23 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG21 | 10 | 0.23 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG22 | 10 | 0.23 |
| (1,1584) | 1:120:A:TYR:HD2 | 1:94:A:ILE:HG23 | 10 | 0.23 |
| (1,1526) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 8 | 0.23 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 3 | 0.23 |
| (1,1448) | 1:85:A:ARG:HD2 | 1:81:A:ASN:HA | 3 | 0.23 |
| (1,1426) | 1:85:A:ARG:HA | 1:87:A:ASN:H | 9 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 1 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 2 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 3 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 4 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 5 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 6 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 7 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 8 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 9 | 0.23 |
| (1,1408) | 1:84:A:TYR:HB2 | 1:84:A:TYR:HA | 10 | 0.23 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 7 | 0.23 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 9 | 0.23 |
| (1,1223) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 7 | 0.23 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 2 | 0.23 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 7 | 0.23 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 9 | 0.23 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 2 | 0.23 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 6 | 0.23 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 6 | 0.23 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 6 | 0.23 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 4 | 0.23 |
| (1,906) | 1:58:A:LYS:H | 1:57:A:ASP:HB2 | 9 | 0.23 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 5 | 0.23 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 1 | 0.23 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 1 | 0.23 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 1 | 0.23 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 1 | 0.23 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 1 | 0.23 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 1 | 0.23 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 7 | 0.23 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 7 | 0.23 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 7 | 0.23 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD11 | 8 | 0.23 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD12 | 8 | 0.23 |
| (1,855) | 1:37:A:ALA:H | 1:53:A:ILE:HD13 | 8 | 0.23 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 9 | 0.23 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 9 | 0.23 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 9 | 0.23 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 3 | 0.23 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 7 | 0.23 |
| (1,699) | 1:43:A:ILE:HG12 | 1:43:A:ILE:HA | 8 | 0.23 |
| (1,683) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HA | 1 | 0.23 |
| (1,683) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HA | 1 | 0.23 |
| (1,683) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HA | 1 | 0.23 |
| (1,683) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HA | 10 | 0.23 |
| (1,683) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HA | 10 | 0.23 |
| (1,683) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HA | 10 | 0.23 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 1 | 0.23 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 1 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 1 | 0.23 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 1 | 0.23 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 1 | 0.23 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 1 | 0.23 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 5 | 0.23 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 5 | 0.23 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 5 | 0.23 |
| (1,375) | 1:23:A:ILE:HG21 | 1:66:A:LEU:HA | 7 | 0.23 |
| (1,375) | 1:23:A:ILE:HG22 | 1:66:A:LEU:HA | 7 | 0.23 |
| (1,375) | 1:23:A:ILE:HG23 | 1:66:A:LEU:HA | 7 | 0.23 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 2 | 0.23 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 2 | 0.23 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 2 | 0.23 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 5 | 0.23 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 5 | 0.23 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 5 | 0.23 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 10 | 0.23 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 10 | 0.23 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 10 | 0.23 |
| (1,74) | 1:11:A:THR:HB | 1:13:A:TYR:H | 4 | 0.23 |
| (3,1183) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 9 | 0.22 |
| (3,1170) | 1:111:A:LYS:HB2 | 1:112:A:GLY:H | 2 | 0.22 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 3 | 0.22 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 10 | 0.22 |
| (3,1030) | 1:53:A:ILE:H | 1:37:A:ALA:H | 10 | 0.22 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 10 | 0.22 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 6 | 0.22 |
| (3,970) | 1:100:A:SER:H | 1:101:A:ALA:H | 10 | 0.22 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG21 | 1 | 0.22 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG22 | 10 | 0.22 |
| (3,885) | 1:69:A:VAL:HG21 | 1:125:A:LYS:HB2 | 5 | 0.22 |
| (3,870) | 1:56:A:GLY:HA3 | 1:57:A:ASP:H | 10 | 0.22 |
| (3,864) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 1 | 0.22 |
| (3,864) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 4 | 0.22 |
| (3,864) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 6 | 0.22 |
| (3,864) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 9 | 0.22 |
| (3,864) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 10 | 0.22 |
| (3,854) | 1:104:A:VAL:HA | 1:103:A:ILE:HB | 7 | 0.22 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 4 | 0.22 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 8 | 0.22 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 9 | 0.22 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD11 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD12 | 2 | 0.22 |
| (3,782) | 1:96:A:GLU:HB2 | 1:94:A:ILE:HD13 | 2 | 0.22 |
| (3,743) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HA | 1 | 0.22 |
| (3,735) | 1:115:A:VAL:HG13 | 1:103:A:ILE:HD12 | 1 | 0.22 |
| (3,680) | 1:23:A:ILE:H | 1:24:A:ILE:HD12 | 6 | 0.22 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 7 | 0.22 |
| (3,598) | 1:52:A:MET:H | 1:52:A:MET:HB3 | 3 | 0.22 |
| (3,595) | 1:105:A:ILE:HB | 1:106:A:GLU:H | 4 | 0.22 |
| (3,583) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB3 | 5 | 0.22 |
| (3,545) | 1:49:A:VAL:HG11 | 1:49:A:VAL:HA | 4 | 0.22 |
| (3,487) | 1:5:A:LYS:HG2 | 1:5:A:LYS:HE3 | 4 | 0.22 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 7 | 0.22 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 6 | 0.22 |
| (3,450) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 10 | 0.22 |
| (3,396) | 1:121:A:GLU:HA | 1:123:A:ILE:HG22 | 2 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 2 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 4 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 5 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 6 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 7 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 8 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 9 | 0.22 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 10 | 0.22 |
| (3,300) | 1:11:A:THR:HG23 | 1:13:A:TYR:HE1 | 5 | 0.22 |
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 5 | 0.22 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG22 | 5 | 0.22 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG23 | 9 | 0.22 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG23 | 10 | 0.22 |
| (3,85) | 1:39:A:VAL:HG23 | 1:50:A:VAL:HA | 4 | 0.22 |
| (3,85) | 1:39:A:VAL:HG22 | 1:50:A:VAL:HA | 8 | 0.22 |
| (2,414) | 1:27:A:LYS:HA | 1:25:A:THR:HB | 10 | 0.22 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 6 | 0.22 |
| (1,3842) | 1:46:A:TYR:HE1 | 1:45:A:LYS:HB2 | 9 | 0.22 |
| (1,3842) | 1:46:A:TYR:HE2 | 1:45:A:LYS:HB2 | 9 | 0.22 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 1 | 0.22 |
| (1,3705) | 1:75:A:LYS:H | 1:91:A:LEU:HA | 4 | 0.22 |
| (1,3696) | 1:68:A:THR:H | 1:14:A:TRP:HZ2 | 2 | 0.22 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 4 | 0.22 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 3 | 0.22 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 6 | 0.22 |
| (1,3499) | 1:37:A:ALA:H | 1:36:A:LYS:HE2 | 5 | 0.22 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 7 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3421) | 1:10:A:ARG:H | 1:82:A:GLY:HA3 | 5 | 0.22 |
| (1,3385) | 1:13:A:TYR:H | 1:12:A:ASP:HB2 | 7 | 0.22 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 8 | 0.22 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 8 | 0.22 |
| (1,3363) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 8 | 0.22 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 3 | 0.22 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 3 | 0.22 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 3 | 0.22 |
| (1,3210) | 1:36:A:LYS:H | 1:36:A:LYS:HE3 | 5 | 0.22 |
| (1,3163) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 2 | 0.22 |
| (1,3163) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 2 | 0.22 |
| (1,3163) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 2 | 0.22 |
| (1,3028) | 1:51:A:LYS:HG2 | 1:56:A:GLY:H | 1 | 0.22 |
| (1,3021) | 1:51:A:LYS:HD2 | 1:57:A:ASP:H | 8 | 0.22 |
| (1,2979) | 1:62:A:ASP:H | 1:65:A:HIS:HD2 | 8 | 0.22 |
| (1,2967) | 1:46:A:TYR:HB2 | 1:63:A:GLN:H | 8 | 0.22 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 9 | 0.22 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD11 | 5 | 0.22 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD12 | 5 | 0.22 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD13 | 5 | 0.22 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 7 | 0.22 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 9 | 0.22 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 10 | 0.22 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 3 | 0.22 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 7 | 0.22 |
| (1,2661) | 1:102:A:THR:H | 1:93:A:SER:H | 6 | 0.22 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 5 | 0.22 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 5 | 0.22 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 5 | 0.22 |
| (1,2604) | 1:95:A:ASN:HB2 | 1:99:A:PHE:H | 2 | 0.22 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 10 | 0.22 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 6 | 0.22 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 6 | 0.22 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 5 | 0.22 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 7 | 0.22 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 8 | 0.22 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 10 | 0.22 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 10 | 0.22 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 10 | 0.22 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 4 | 0.22 |
| (1,2461) | 1:84:A:TYR:HE1 | 1:113:A:ARG:H | 8 | 0.22 |
| (1,2461) | 1:84:A:TYR:HE2 | 1:113:A:ARG:H | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 8 | 0.22 |
| (1,2448) | 1:115:A:VAL:H | 1:103:A:ILE:HG13 | 3 | 0.22 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 2 | 0.22 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 6 | 0.22 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 1 | 0.22 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 8 | 0.22 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 9 | 0.22 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 5 | 0.22 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 3 | 0.22 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 3 | 0.22 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 3 | 0.22 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 5 | 0.22 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 5 | 0.22 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 5 | 0.22 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 8 | 0.22 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 8 | 0.22 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 8 | 0.22 |
| (1,2137) | 1:119:A:GLN:HG2 | 1:100:A:SER:HB2 | 7 | 0.22 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 4 | 0.22 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 4 | 0.22 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 4 | 0.22 |
| (1,1938) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 3 | 0.22 |
| (1,1922) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD2 | 8 | 0.22 |
| (1,1922) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD2 | 8 | 0.22 |
| (1,1922) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD2 | 8 | 0.22 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 4 | 0.22 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 4 | 0.22 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 4 | 0.22 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD21 | 10 | 0.22 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD22 | 10 | 0.22 |
| (1,1887) | 1:76:A:ARG:HD3 | 1:126:A:LEU:HD23 | 10 | 0.22 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD11 | 8 | 0.22 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD12 | 8 | 0.22 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD13 | 8 | 0.22 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 8 | 0.22 |
| (1,1657) | 1:101:A:ALA:HB1 | 1:95:A:ASN:H | 2 | 0.22 |
| (1,1657) | 1:101:A:ALA:HB2 | 1:95:A:ASN:H | 2 | 0.22 |
| (1,1657) | 1:101:A:ALA:HB3 | 1:95:A:ASN:H | 2 | 0.22 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 8 | 0.22 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 8 | 0.22 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 8 | 0.22 |
| (1,1555) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 7 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 6 | 0.22 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD11 | 1 | 0.22 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD12 | 1 | 0.22 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD13 | 1 | 0.22 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 2 | 0.22 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 4 | 0.22 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 6 | 0.22 |
| (1,1223) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 6 | 0.22 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 8 | 0.22 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 7 | 0.22 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 7 | 0.22 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 7 | 0.22 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 4 | 0.22 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 4 | 0.22 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 4 | 0.22 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 4 | 0.22 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 6 | 0.22 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 4 | 0.22 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 4 | 0.22 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 8 | 0.22 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 1 | 0.22 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 1 | 0.22 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 1 | 0.22 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 6 | 0.22 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 7 | 0.22 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 7 | 0.22 |
| (1,832) | 1:52:A:MET:H | 1:52:A:MET:HG2 | 7 | 0.22 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 8 | 0.22 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 8 | 0.22 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 8 | 0.22 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 5 | 0.22 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 5 | 0.22 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 5 | 0.22 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 4 | 0.22 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 4 | 0.22 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 4 | 0.22 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 8 | 0.22 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 8 | 0.22 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 8 | 0.22 |
| (1,458) | 1:61:A:LEU:HD21 | 1:60:A:LYS:H | 2 | 0.22 |
| (1,458) | 1:61:A:LEU:HD22 | 1:60:A:LYS:H | 2 | 0.22 |
| (1,458) | 1:61:A:LEU:HD23 | 1:60:A:LYS:H | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1182) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 8 | 0.21 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 6 | 0.21 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 7 | 0.21 |
| (3,931) | 1:124:A:SER:HB3 | 1:123:A:ILE:HG23 | 10 | 0.21 |
| (3,890) | 1:78:A:LEU:HA | 1:124:A:SER:H | 1 | 0.21 |
| (3,864) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 3 | 0.21 |
| (3,864) | 1:53:A:ILE:HG22 | 1:53:A:ILE:HB | 5 | 0.21 |
| (3,864) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 7 | 0.21 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 1 | 0.21 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 6 | 0.21 |
| (3,545) | 1:49:A:VAL:HG13 | 1:49:A:VAL:HA | 2 | 0.21 |
| (3,545) | 1:49:A:VAL:HG13 | 1:49:A:VAL:HA | 5 | 0.21 |
| (3,487) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HG3 | 3 | 0.21 |
| (3,440) | 1:103:A:ILE:H | 1:117:A:GLY:H | 5 | 0.21 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 9 | 0.21 |
| (3,388) | 1:73:A:PRO:HB2 | 1:73:A:PRO:HA | 3 | 0.21 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 10 | 0.21 |
| (3,353) | 1:61:A:LEU:HD22 | 1:61:A:LEU:HB3 | 9 | 0.21 |
| (3,353) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HB3 | 10 | 0.21 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 8 | 0.21 |
| (3,139) | 1:85:A:ARG:HA | 1:79:A:VAL:HG13 | 9 | 0.21 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG23 | 1 | 0.21 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 6 | 0.21 |
| (2,609) | 1:119:A:GLN:HE21 | 1:121:A:GLU:HB2 | 9 | 0.21 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 9 | 0.21 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 9 | 0.21 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 9 | 0.21 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG11 | 4 | 0.21 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG12 | 4 | 0.21 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG13 | 4 | 0.21 |
| (2,11) | 1:9:A:ALA:HA | 1:14:A:TRP:HA | 3 | 0.21 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 8 | 0.21 |
| (1,3737) | 1:5:A:LYS:H | 1:3:A:GLU:H | 4 | 0.21 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 8 | 0.21 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 1 | 0.21 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 10 | 0.21 |
| (1,3493) | 1:26:A:LYS:HB2 | 1:33:A:HIS:H | 5 | 0.21 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 2 | 0.21 |
| (1,3468) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HE21 | 1 | 0.21 |
| (1,3468) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HE21 | 1 | 0.21 |
| (1,3468) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HE21 | 1 | 0.21 |
| (1,3449) | 1:15:A:LEU:H | 1:14:A:TRP:HE1 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3434) | 1:63:A:GLN:HE22 | 1:14:A:TRP:HE1 | 9 | 0.21 |
| (1,3395) | 1:11:A:THR:H | 1:81:A:ASN:HB3 | 5 | 0.21 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 1 | 0.21 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 1 | 0.21 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 1 | 0.21 |
| (1,3268) | 1:32:A:TYR:HD1 | 1:29:A:GLY:H | 6 | 0.21 |
| (1,3268) | 1:32:A:TYR:HD2 | 1:29:A:GLY:H | 6 | 0.21 |
| (1,3245) | 1:30:A:GLU:HG3 | 1:33:A:HIS:H | 9 | 0.21 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 6 | 0.21 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 6 | 0.21 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 6 | 0.21 |
| (1,3146) | 1:42:A:VAL:HG21 | 1:43:A:ILE:H | 10 | 0.21 |
| (1,3146) | 1:42:A:VAL:HG22 | 1:43:A:ILE:H | 10 | 0.21 |
| (1,3146) | 1:42:A:VAL:HG23 | 1:43:A:ILE:H | 10 | 0.21 |
| (1,3134) | 1:44:A:ASP:H | 1:43:A:ILE:HG13 | 3 | 0.21 |
| (1,3128) | 1:47:A:THR:HB | 1:44:A:ASP:H | 8 | 0.21 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 4 | 0.21 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 4 | 0.21 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 4 | 0.21 |
| (1,3021) | 1:51:A:LYS:HD2 | 1:57:A:ASP:H | 9 | 0.21 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 2 | 0.21 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 10 | 0.21 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 2 | 0.21 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 8 | 0.21 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 8 | 0.21 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 5 | 0.21 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 1 | 0.21 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 4 | 0.21 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 4 | 0.21 |
| (1,2436) | 1:115:A:VAL:HB | 1:116:A:GLU:H | 1 | 0.21 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 2 | 0.21 |
| (1,2404) | 1:119:A:GLN:HB3 | 1:119:A:GLN:H | 8 | 0.21 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 9 | 0.21 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 4 | 0.21 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 8 | 0.21 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 1 | 0.21 |
| (1,2285) | 1:20:A:ILE:HA | 1:20:A:ILE:HG12 | 5 | 0.21 |
| (1,2285) | 1:20:A:ILE:HA | 1:20:A:ILE:HG12 | 6 | 0.21 |
| (1,2285) | 1:20:A:ILE:HA | 1:20:A:ILE:HG12 | 7 | 0.21 |
| (1,2285) | 1:20:A:ILE:HA | 1:20:A:ILE:HG12 | 10 | 0.21 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 7 | 0.21 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 7 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 7 | 0.21 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 6 | 0.21 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 6 | 0.21 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 6 | 0.21 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 1 | 0.21 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 1 | 0.21 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 1 | 0.21 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 8 | 0.21 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 8 | 0.21 |
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 8 | 0.21 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 5 | 0.21 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 5 | 0.21 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 5 | 0.21 |
| (1,2102) | 1:126:A:LEU:HD21 | 1:77:A:ILE:H | 8 | 0.21 |
| (1,2102) | 1:126:A:LEU:HD22 | 1:77:A:ILE:H | 8 | 0.21 |
| (1,2102) | 1:126:A:LEU:HD23 | 1:77:A:ILE:H | 8 | 0.21 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 5 | 0.21 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 5 | 0.21 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 5 | 0.21 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 9 | 0.21 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 9 | 0.21 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 9 | 0.21 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 9 | 0.21 |
| (1,1777) | 1:106:A:GLU:HB3 | 1:106:A:GLU:H | 6 | 0.21 |
| (1,1762) | 1:105:A:ILE:HG21 | 1:106:A:GLU:HA | 6 | 0.21 |
| (1,1762) | 1:105:A:ILE:HG22 | 1:106:A:GLU:HA | 6 | 0.21 |
| (1,1762) | 1:105:A:ILE:HG23 | 1:106:A:GLU:HA | 6 | 0.21 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 10 | 0.21 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 10 | 0.21 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 10 | 0.21 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG21 | 9 | 0.21 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG22 | 9 | 0.21 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG23 | 9 | 0.21 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 1 | 0.21 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 2 | 0.21 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 3 | 0.21 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 6 | 0.21 |
| (1,1716) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 10 | 0.21 |
| (1,1716) | 1:103:A:ILE:HG22 | 1:102:A:THR:HA | 10 | 0.21 |
| (1,1716) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 10 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 1 | 0.21 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 1 | 0.21 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 3 | 0.21 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 6 | 0.21 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 8 | 0.21 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 9 | 0.21 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 4 | 0.21 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 4 | 0.21 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 4 | 0.21 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 2 | 0.21 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 2 | 0.21 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 2 | 0.21 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG21 | 6 | 0.21 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG22 | 6 | 0.21 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG23 | 6 | 0.21 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 6 | 0.21 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 10 | 0.21 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 6 | 0.21 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 5 | 0.21 |
| (1,906) | 1:58:A:LYS:H | 1:57:A:ASP:HB2 | 5 | 0.21 |
| (1,900) | 1:57:A:ASP:HA | 1:57:A:ASP:HB3 | 6 | 0.21 |
| (1,900) | 1:57:A:ASP:HA | 1:57:A:ASP:HB3 | 8 | 0.21 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 4 | 0.21 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 4 | 0.21 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 4 | 0.21 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 7 | 0.21 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 7 | 0.21 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 7 | 0.21 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 2 | 0.21 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 3 | 0.21 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 5 | 0.21 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 1 | 0.21 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 1 | 0.21 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 1 | 0.21 |
| (1,574) | 1:39:A:VAL:HG11 | 1:40:A:LYS:H | 5 | 0.21 |
| (1,574) | 1:39:A:VAL:HG12 | 1:40:A:LYS:H | 5 | 0.21 |
| (1,574) | 1:39:A:VAL:HG13 | 1:40:A:LYS:H | 5 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,571) | 1:39:A:VAL:HG11 | 1:50:A:VAL:HA | 6 | 0.21 |
| (1,571) | 1:39:A:VAL:HG12 | 1:50:A:VAL:HA | 6 | 0.21 |
| (1,571) | 1:39:A:VAL:HG13 | 1:50:A:VAL:HA | 6 | 0.21 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 10 | 0.21 |
| (1,458) | 1:61:A:LEU:HD21 | 1:60:A:LYS:H | 4 | 0.21 |
| (1,458) | 1:61:A:LEU:HD22 | 1:60:A:LYS:H | 4 | 0.21 |
| (1,458) | 1:61:A:LEU:HD23 | 1:60:A:LYS:H | 4 | 0.21 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 10 | 0.21 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 10 | 0.21 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 10 | 0.21 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 10 | 0.21 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 10 | 0.21 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 10 | 0.21 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 4 | 0.21 |
| (1,390) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 5 | 0.21 |
| (1,390) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 5 | 0.21 |
| (1,390) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 5 | 0.21 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 8 | 0.21 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 8 | 0.21 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 8 | 0.21 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 3 | 0.21 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 3 | 0.21 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 3 | 0.21 |
| (1,143) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 8 | 0.21 |
| (1,143) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 8 | 0.21 |
| (1,143) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 8 | 0.21 |
| (3,1087) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HB3 | 3 | 0.2 |
| (3,1087) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HB3 | 3 | 0.2 |
| (3,1087) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HB3 | 3 | 0.2 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 9 | 0.2 |
| (3,988) | 1:96:A:GLU:HA | 1:99:A:PHE:H | 6 | 0.2 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 4 | 0.2 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG21 | 3 | 0.2 |
| (3,890) | 1:68:A:THR:HB | 1:124:A:SER:H | 3 | 0.2 |
| (3,885) | 1:69:A:VAL:HG23 | 1:125:A:LYS:HB2 | 2 | 0.2 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 5 | 0.2 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 7 | 0.2 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 10 | 0.2 |
| (3,815) | 1:123:A:ILE:HG12 | 1:123:A:ILE:HA | 3 | 0.2 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 1 | 0.2 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 4 | 0.2 |
| (3,743) | 1:37:A:ALA:HB3 | 1:50:A:VAL:HA | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,595) | 1:106:A:GLU:HG3 | 1:106:A:GLU:H | 9 | 0.2 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 1 | 0.2 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 2 | 0.2 |
| (3,487) | 1:5:A:LYS:HE2 | 1:5:A:LYS:HG3 | 5 | 0.2 |
| (3,423) | 1:61:A:LEU:HD11 | 1:25:A:THR:H | 3 | 0.2 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 6 | 0.2 |
| (3,366) | 1:42:A:VAL:HG23 | 1:16:A:GLN:HG2 | 4 | 0.2 |
| (3,353) | 1:61:A:LEU:HD21 | 1:61:A:LEU:HB3 | 3 | 0.2 |
| (3,345) | 1:35:A:LYS:H | 1:22:A:LYS:HG3 | 4 | 0.2 |
| (3,180) | 1:65:A:HIS:H | 1:62:A:ASP:HB3 | 2 | 0.2 |
| (3,180) | 1:65:A:HIS:H | 1:62:A:ASP:HB3 | 3 | 0.2 |
| (3,177) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HA | 3 | 0.2 |
| (3,121) | 1:38:A:ILE:HB | 1:38:A:ILE:HG21 | 8 | 0.2 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 7 | 0.2 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 8 | 0.2 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 9 | 0.2 |
| (3,4) | 1:102:A:THR:HG23 | 1:116:A:GLU:H | 4 | 0.2 |
| (2,386) | 1:95:A:ASN:HB2 | 1:99:A:PHE:HA | 1 | 0.2 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG11 | 6 | 0.2 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG12 | 6 | 0.2 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG13 | 6 | 0.2 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 4 | 0.2 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 4 | 0.2 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 10 | 0.2 |
| (1,3779) | 1:46:A:TYR:HD1 | 1:63:A:GLN:HG3 | 5 | 0.2 |
| (1,3779) | 1:46:A:TYR:HD2 | 1:63:A:GLN:HG3 | 5 | 0.2 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 5 | 0.2 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 5 | 0.2 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 6 | 0.2 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 6 | 0.2 |
| (1,3759) | 1:27:A:LYS:HG3 | 1:65:A:HIS:HE1 | 3 | 0.2 |
| (1,3752) | 1:34:A:LYS:HG2 | 1:33:A:HIS:HE1 | 7 | 0.2 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 6 | 0.2 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 1 | 0.2 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 2 | 0.2 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 4 | 0.2 |
| (1,3560) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 7 | 0.2 |
| (1,3556) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 10 | 0.2 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 10 | 0.2 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 3 | 0.2 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 4 | 0.2 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3397) | 1:10:A:ARG:HB3 | 1:11:A:THR:H | 4 | 0.2 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 2 | 0.2 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB3 | 5 | 0.2 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 5 | 0.2 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 7 | 0.2 |
| (1,2898) | 1:69:A:VAL:H | 1:69:A:VAL:HB | 6 | 0.2 |
| (1,2843) | 1:105:A:ILE:HG21 | 1:112:A:GLY:H | 2 | 0.2 |
| (1,2843) | 1:105:A:ILE:HG22 | 1:112:A:GLY:H | 2 | 0.2 |
| (1,2843) | 1:105:A:ILE:HG23 | 1:112:A:GLY:H | 2 | 0.2 |
| (1,2831) | 1:78:A:LEU:H | 1:123:A:ILE:HB | 6 | 0.2 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 3 | 0.2 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 9 | 0.2 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 9 | 0.2 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 9 | 0.2 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 5 | 0.2 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 9 | 0.2 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 1 | 0.2 |
| (1,2590) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 3 | 0.2 |
| (1,2573) | 1:101:A:ALA:H | 1:100:A:SER:HB2 | 4 | 0.2 |
| (1,2494) | 1:108:A:GLY:H | 1:111:A:LYS:HE3 | 6 | 0.2 |
| (1,2473) | 1:105:A:ILE:HD11 | 1:111:A:LYS:H | 10 | 0.2 |
| (1,2473) | 1:105:A:ILE:HD12 | 1:111:A:LYS:H | 10 | 0.2 |
| (1,2473) | 1:105:A:ILE:HD13 | 1:111:A:LYS:H | 10 | 0.2 |
| (1,2461) | 1:84:A:TYR:HE1 | 1:113:A:ARG:H | 7 | 0.2 |
| (1,2461) | 1:84:A:TYR:HE2 | 1:113:A:ARG:H | 7 | 0.2 |
| (1,2459) | 1:113:A:ARG:H | 1:107:A:THR:H | 8 | 0.2 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 4 | 0.2 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 5 | 0.2 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 8 | 0.2 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 6 | 0.2 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 9 | 0.2 |
| (1,2285) | 1:20:A:ILE:HA | 1:20:A:ILE:HG12 | 1 | 0.2 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 7 | 0.2 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 7 | 0.2 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 7 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 2 | 0.2 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 2 | 0.2 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 5 | 0.2 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 5 | 0.2 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 5 | 0.2 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 9 | 0.2 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 9 | 0.2 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 9 | 0.2 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 9 | 0.2 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 9 | 0.2 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 9 | 0.2 |
| (1,2197) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 3 | 0.2 |
| (1,2157) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB3 | 7 | 0.2 |
| (1,2148) | 1:93:A:SER:H | 1:91:A:LEU:HG | 9 | 0.2 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 3 | 0.2 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 3 | 0.2 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 3 | 0.2 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG21 | 7 | 0.2 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG22 | 7 | 0.2 |
| (1,2122) | 1:78:A:LEU:HA | 1:123:A:ILE:HG23 | 7 | 0.2 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 7 | 0.2 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 5 | 0.2 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 10 | 0.2 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 4 | 0.2 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 4 | 0.2 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 4 | 0.2 |
| (1,1738) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 6 | 0.2 |
| (1,1738) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 6 | 0.2 |
| (1,1738) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 6 | 0.2 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 7 | 0.2 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 10 | 0.2 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 1 | 0.2 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 5 | 0.2 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 7 | 0.2 |
| (1,1590) | 1:95:A:ASN:HD22 | 1:95:A:ASN:HB2 | 10 | 0.2 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 4 | 0.2 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 7 | 0.2 |
| (1,1352) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA2 | 5 | 0.2 |
| (1,1352) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA2 | 5 | 0.2 |
| (1,1352) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA2 | 5 | 0.2 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 5 | 0.2 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 9 | 0.2 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 9 | 0.2 |
| (1,1301) | 1:125:A:LYS:HA | 1:77:A:ILE:HB | 10 | 0.2 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 10 | 0.2 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 9 | 0.2 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 1 | 0.2 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 1 | 0.2 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 1 | 0.2 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 8 | 0.2 |
| (1,1021) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 10 | 0.2 |
| (1,1021) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 10 | 0.2 |
| (1,1021) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 10 | 0.2 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 1 | 0.2 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 5 | 0.2 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 9 | 0.2 |
| (1,900) | 1:57:A:ASP:HA | 1:57:A:ASP:HB3 | 5 | 0.2 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 9 | 0.2 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 1 | 0.2 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 7 | 0.2 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 6 | 0.2 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 6 | 0.2 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 6 | 0.2 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 2 | 0.2 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 2 | 0.2 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 2 | 0.2 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 7 | 0.2 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 7 | 0.2 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 7 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 4 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 4 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 4 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 7 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 7 | 0.2 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 7 | 0.2 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG11 | 6 | 0.2 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG12 | 6 | 0.2 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG13 | 6 | 0.2 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 4 | 0.2 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 4 | 0.2 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 4 | 0.2 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 9 | 0.2 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 9 | 0.2 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 1 | 0.2 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 1 | 0.2 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 1 | 0.2 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 2 | 0.2 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 2 | 0.2 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 2 | 0.2 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 3 | 0.2 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 3 | 0.2 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 3 | 0.2 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 9 | 0.2 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 9 | 0.2 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 9 | 0.2 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD11 | 4 | 0.2 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD12 | 4 | 0.2 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD13 | 4 | 0.2 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 10 | 0.2 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 10 | 0.2 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 10 | 0.2 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 7 | 0.2 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 7 | 0.2 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 7 | 0.2 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HG2 | 5 | 0.19 |
| (3,1128) | 1:72:A:ALA:H | 1:71:A:PRO:HB3 | 1 | 0.19 |
| (3,1076) | 1:97:A:LYS:H | 1:97:A:LYS:HD2 | 3 | 0.19 |
| (3,816) | 1:77:A:ILE:H | 1:91:A:LEU:H | 6 | 0.19 |
| (3,595) | 1:106:A:GLU:HG3 | 1:106:A:GLU:H | 8 | 0.19 |
| (3,545) | 1:49:A:VAL:HG13 | 1:49:A:VAL:HA | 9 | 0.19 |
| (3,523) | 1:20:A:ILE:HG22 | 1:127:A:ALA:HA | 6 | 0.19 |
| (3,487) | 1:6:A:LYS:HG3 | 1:6:A:LYS:HE2 | 8 | 0.19 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 5 | 0.19 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 1 | 0.19 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 4 | 0.19 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 5 | 0.19 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 5 | 0.19 |
| (3,167) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 2 | 0.19 |
| (3,153) | 1:91:A:LEU:HD11 | 1:102:A:THR:H | 9 | 0.19 |
| (3,140) | 1:24:A:ILE:HG21 | 1:67:A:GLU:HG2 | 4 | 0.19 |
| (3,133) | 1:100:A:SER:H | 1:99:A:PHE:HB2 | 6 | 0.19 |
| (3,128) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HG23 | 9 | 0.19 |
| (3,109) | 1:3:A:GLU:HB3 | 1:3:A:GLU:HG2 | 1 | 0.19 |
| (3,107) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HE2 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,43) | 1:77:A:ILE:H | 1:77:A:ILE:HD13 | 3 | 0.19 |
| (3,23) | 1:127:A:ALA:HB1 | 1:18:A:GLU:H | 7 | 0.19 |
| (3,1) | 1:19:A:ILE:HA | 1:19:A:ILE:HG13 | 8 | 0.19 |
| (2,617) | 1:24:A:ILE:HA | 1:33:A:HIS:H | 4 | 0.19 |
| (2,609) | 1:119:A:GLN:HE21 | 1:121:A:GLU:HB2 | 10 | 0.19 |
| (2,608) | 1:89:A:GLY:H | 1:107:A:THR:H | 6 | 0.19 |
| (2,362) | 1:84:A:TYR:HB3 | 1:103:A:ILE:HG13 | 5 | 0.19 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 2 | 0.19 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 4 | 0.19 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 6 | 0.19 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 7 | 0.19 |
| (1,3753) | 1:34:A:LYS:HD2 | 1:33:A:HIS:HE1 | 7 | 0.19 |
| (1,3718) | 1:87:A:ASN:HD21 | 1:79:A:VAL:HB | 7 | 0.19 |
| (1,3715) | 1:84:A:TYR:HE1 | 1:87:A:ASN:HD22 | 8 | 0.19 |
| (1,3715) | 1:84:A:TYR:HE2 | 1:87:A:ASN:HD22 | 8 | 0.19 |
| (1,3695) | 1:68:A:THR:H | 1:121:A:GLU:HB2 | 5 | 0.19 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 1 | 0.19 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 2 | 0.19 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 10 | 0.19 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 10 | 0.19 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 10 | 0.19 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 10 | 0.19 |
| (1,3485) | 1:23:A:ILE:H | 1:33:A:HIS:HA | 6 | 0.19 |
| (1,3391) | 1:11:A:THR:H | 1:81:A:ASN:HD22 | 3 | 0.19 |
| (1,3243) | 1:30:A:GLU:HB3 | 1:33:A:HIS:H | 2 | 0.19 |
| (1,3208) | 1:36:A:LYS:HG2 | 1:36:A:LYS:H | 5 | 0.19 |
| (1,3133) | 1:44:A:ASP:H | 1:43:A:ILE:HG12 | 3 | 0.19 |
| (1,3128) | 1:47:A:THR:HB | 1:44:A:ASP:H | 7 | 0.19 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 3 | 0.19 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 6 | 0.19 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 10 | 0.19 |
| (1,2869) | 1:91:A:LEU:HB2 | 1:74:A:GLY:H | 10 | 0.19 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 2 | 0.19 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 2 | 0.19 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 4 | 0.19 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 1 | 0.19 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 5 | 0.19 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 10 | 0.19 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 4 | 0.19 |
| (1,2633) | 1:96:A:GLU:H | 1:95:A:ASN:HB3 | 7 | 0.19 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 7 | 0.19 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 5 | 0.19 |
| (1,2565) | 1:117:A:GLY:H | 1:101:A:ALA:H | 4 | 0.19 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 3 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 4 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 4 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 4 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 5 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 5 | 0.19 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 5 | 0.19 |
| (1,2447) | 1:115:A:VAL:HB | 1:115:A:VAL:H | 3 | 0.19 |
| (1,2447) | 1:115:A:VAL:HB | 1:115:A:VAL:H | 5 | 0.19 |
| (1,2442) | 1:103:A:ILE:H | 1:116:A:GLU:H | 10 | 0.19 |
| (1,2382) | 1:120:A:TYR:H | 1:119:A:GLN:HB2 | 4 | 0.19 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 2 | 0.19 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 10 | 0.19 |
| (1,2275) | 1:21:A:VAL:HG21 | 1:22:A:LYS:H | 2 | 0.19 |
| (1,2275) | 1:21:A:VAL:HG22 | 1:22:A:LYS:H | 2 | 0.19 |
| (1,2275) | 1:21:A:VAL:HG23 | 1:22:A:LYS:H | 2 | 0.19 |
| (1,2271) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HA | 9 | 0.19 |
| (1,2271) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HA | 9 | 0.19 |
| (1,2271) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HA | 9 | 0.19 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 8 | 0.19 |
| (1,2251) | 1:60:A:LYS:HE2 | 1:49:A:VAL:HA | 7 | 0.19 |
| (1,2221) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HA | 2 | 0.19 |
| (1,2221) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HA | 2 | 0.19 |
| (1,2221) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 2 | 0.19 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 3 | 0.19 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 3 | 0.19 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 3 | 0.19 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 5 | 0.19 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 5 | 0.19 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 5 | 0.19 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 5 | 0.19 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 5 | 0.19 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 5 | 0.19 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 6 | 0.19 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 6 | 0.19 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 6 | 0.19 |
| (1,2047) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 6 | 0.19 |
| (1,2047) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 6 | 0.19 |
| (1,2047) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 6 | 0.19 |
| (1,1966) | 1:118:A:ILE:HG21 | 1:122:A:ASP:H | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1966) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 1 | 0.19 |
| (1,1966) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 1 | 0.19 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 5 | 0.19 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 6 | 0.19 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 8 | 0.19 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 7 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD11 | 2 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD12 | 2 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD13 | 2 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD11 | 9 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD12 | 9 | 0.19 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD13 | 9 | 0.19 |
| (1,1777) | 1:106:A:GLU:HB3 | 1:106:A:GLU:H | 3 | 0.19 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 1 | 0.19 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 1 | 0.19 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 1 | 0.19 |
| (1,1731) | 1:105:A:ILE:HG13 | 1:105:A:ILE:HA | 9 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 7 | 0.19 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 7 | 0.19 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 2 | 0.19 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 3 | 0.19 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 10 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 3 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 4 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 5 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 7 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 8 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 9 | 0.19 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 10 | 0.19 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 10 | 0.19 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 7 | 0.19 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 7 | 0.19 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 7 | 0.19 |
| (1,1454) | 1:78:A:LEU:HD21 | 1:86:A:GLY:HA2 | 6 | 0.19 |
| (1,1454) | 1:78:A:LEU:HD22 | 1:86:A:GLY:HA2 | 6 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1454) | 1:78:A:LEU:HD23 | 1:86:A:GLY:HA2 | 6 | 0.19 |
| (1,1453) | 1:78:A:LEU:HD21 | 1:86:A:GLY:HA2 | 6 | 0.19 |
| (1,1453) | 1:78:A:LEU:HD22 | 1:86:A:GLY:HA2 | 6 | 0.19 |
| (1,1453) | 1:78:A:LEU:HD23 | 1:86:A:GLY:HA2 | 6 | 0.19 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 10 | 0.19 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 10 | 0.19 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 10 | 0.19 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG21 | 8 | 0.19 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG22 | 8 | 0.19 |
| (1,1316) | 1:126:A:LEU:H | 1:77:A:ILE:HG23 | 8 | 0.19 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 2 | 0.19 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 2 | 0.19 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 2 | 0.19 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 6 | 0.19 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 6 | 0.19 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 6 | 0.19 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 7 | 0.19 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 7 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 2 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 2 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 2 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 5 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 5 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 5 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 8 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 8 | 0.19 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 8 | 0.19 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 8 | 0.19 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 7 | 0.19 |
| (1,1003) | 1:62:A:ASP:HB2 | 1:64:A:THR:HG21 | 1 | 0.19 |
| (1,1003) | 1:62:A:ASP:HB2 | 1:64:A:THR:HG22 | 1 | 0.19 |
| (1,1003) | 1:62:A:ASP:HB2 | 1:64:A:THR:HG23 | 1 | 0.19 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 8 | 0.19 |
| (1,896) | 1:51:A:LYS:HE2 | 1:56:A:GLY:HA2 | 7 | 0.19 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 6 | 0.19 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 8 | 0.19 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 3 | 0.19 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 6 | 0.19 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 6 | 0.19 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 6 | 0.19 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 10 | 0.19 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 10 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 10 | 0.19 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 6 | 0.19 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 6 | 0.19 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 6 | 0.19 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 5 | 0.19 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 5 | 0.19 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 5 | 0.19 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB1 | 1 | 0.19 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB2 | 1 | 0.19 |
| (1,531) | 1:53:A:ILE:H | 1:37:A:ALA:HB3 | 1 | 0.19 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD11 | 3 | 0.19 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD12 | 3 | 0.19 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD13 | 3 | 0.19 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 10 | 0.19 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 10 | 0.19 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 10 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG21 | 3 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG22 | 3 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG23 | 3 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG21 | 9 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG22 | 9 | 0.19 |
| (1,270) | 1:126:A:LEU:HA | 1:19:A:ILE:HG23 | 9 | 0.19 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 8 | 0.19 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 8 | 0.19 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 8 | 0.19 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 9 | 0.19 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 9 | 0.19 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 9 | 0.19 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG21 | 6 | 0.19 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG22 | 6 | 0.19 |
| (1,178) | 1:17:A:PRO:HA | 1:39:A:VAL:HG23 | 6 | 0.19 |
| (3,1182) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 1 | 0.18 |
| (3,1146) | 1:115:A:VAL:HA | 1:103:A:ILE:H | 5 | 0.18 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG22 | 5 | 0.18 |
| (3,1057) | 1:8:A:THR:HB | 1:8:A:THR:HG22 | 5 | 0.18 |
| (3,1057) | 1:8:A:THR:HB | 1:8:A:THR:HG21 | 7 | 0.18 |
| (3,993) | 1:61:A:LEU:HG | 1:50:A:VAL:H | 1 | 0.18 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 5 | 0.18 |
| (3,973) | 1:20:A:ILE:HG23 | 1:21:A:VAL:H | 8 | 0.18 |
| (3,644) | 1:3:A:GLU:HA | 1:4:A:GLU:H | 9 | 0.18 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 8 | 0.18 |
| (3,545) | 1:49:A:VAL:HG13 | 1:49:A:VAL:HA | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,545) | 1:49:A:VAL:HG11 | 1:49:A:VAL:HA | 10 | 0.18 |
| (3,537) | 1:85:A:ARG:HD2 | 1:82:A:GLY:H | 2 | 0.18 |
| (3,487) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HB | 2 | 0.18 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 1 | 0.18 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 6 | 0.18 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 7 | 0.18 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 8 | 0.18 |
| (3,396) | 1:118:A:ILE:HG22 | 1:121:A:GLU:HA | 3 | 0.18 |
| (3,348) | 1:113:A:ARG:H | 1:113:A:ARG:HD2 | 7 | 0.18 |
| (3,280) | 1:112:A:GLY:H | 1:111:A:LYS:HG3 | 5 | 0.18 |
| (3,186) | 1:59:A:LEU:H | 1:57:A:ASP:HB2 | 7 | 0.18 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 5 | 0.18 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 9 | 0.18 |
| (3,122) | 1:44:A:ASP:HB3 | 1:43:A:ILE:HG21 | 5 | 0.18 |
| (3,58) | 1:23:A:ILE:HG21 | 1:24:A:ILE:H | 5 | 0.18 |
| (3,52) | 1:6:A:LYS:H | 1:6:A:LYS:HB2 | 6 | 0.18 |
| (2,650) | 1:61:A:LEU:HB2 | 1:65:A:HIS:HD2 | 1 | 0.18 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 1 | 0.18 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 3 | 0.18 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 5 | 0.18 |
| (1,3792) | 1:14:A:TRP:HD1 | 1:14:A:TRP:HB2 | 9 | 0.18 |
| (1,3789) | 1:63:A:GLN:HE21 | 1:14:A:TRP:HD1 | 3 | 0.18 |
| (1,3782) | 1:11:A:THR:HB | 1:13:A:TYR:HD1 | 3 | 0.18 |
| (1,3782) | 1:11:A:THR:HB | 1:13:A:TYR:HD2 | 3 | 0.18 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD1 | 5 | 0.18 |
| (1,3778) | 1:45:A:LYS:HB3 | 1:46:A:TYR:HD2 | 5 | 0.18 |
| (1,3726) | 1:95:A:ASN:HD21 | 1:98:A:THR:HB | 3 | 0.18 |
| (1,3641) | 1:11:A:THR:H | 1:81:A:ASN:HD21 | 2 | 0.18 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 8 | 0.18 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 6 | 0.18 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 6 | 0.18 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 6 | 0.18 |
| (1,3537) | 1:46:A:TYR:HE1 | 1:63:A:GLN:HE21 | 4 | 0.18 |
| (1,3537) | 1:46:A:TYR:HE2 | 1:63:A:GLN:HE21 | 4 | 0.18 |
| (1,3509) | 1:40:A:LYS:HE3 | 1:41:A:GLU:H | 1 | 0.18 |
| (1,3493) | 1:26:A:LYS:HB2 | 1:33:A:HIS:H | 10 | 0.18 |
| (1,3403) | 1:10:A:ARG:HD2 | 1:10:A:ARG:H | 2 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 4 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 4 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 4 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 6 | 0.18 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 6 | 0.18 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 4 | 0.18 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 8 | 0.18 |
| (1,3255) | 1:31:A:LYS:HG3 | 1:32:A:TYR:H | 1 | 0.18 |
| (1,3245) | 1:30:A:GLU:HG2 | 1:33:A:HIS:H | 10 | 0.18 |
| (1,3243) | 1:30:A:GLU:HB2 | 1:33:A:HIS:H | 7 | 0.18 |
| (1,3133) | 1:44:A:ASP:H | 1:43:A:ILE:HG12 | 7 | 0.18 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 1 | 0.18 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 1 | 0.18 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 1 | 0.18 |
| (1,3104) | 1:45:A:LYS:HB2 | 1:47:A:THR:H | 9 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 6 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 6 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 6 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 7 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 7 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 7 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 9 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 9 | 0.18 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 9 | 0.18 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 4 | 0.18 |
| (1,2843) | 1:105:A:ILE:HG21 | 1:112:A:GLY:H | 8 | 0.18 |
| (1,2843) | 1:105:A:ILE:HG22 | 1:112:A:GLY:H | 8 | 0.18 |
| (1,2843) | 1:105:A:ILE:HG23 | 1:112:A:GLY:H | 8 | 0.18 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 9 | 0.18 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 10 | 0.18 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 8 | 0.18 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 4 | 0.18 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 1 | 0.18 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 8 | 0.18 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 9 | 0.18 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 2 | 0.18 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 2 | 0.18 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 2 | 0.18 |
| (1,2447) | 1:115:A:VAL:HB | 1:115:A:VAL:H | 1 | 0.18 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 1 | 0.18 |
| (1,2364) | 1:119:A:GLN:HB2 | 1:121:A:GLU:H | 6 | 0.18 |
| (1,2339) | 1:77:A:ILE:HA | 1:124:A:SER:H | 4 | 0.18 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 3 | 0.18 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 7 | 0.18 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 4 | 0.18 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 4 | 0.18 |
| (1,2137) | 1:119:A:GLN:HG2 | 1:100:A:SER:HB2 | 4 | 0.18 |
| (1,2124) | 1:123:A:ILE:HD11 | 1:101:A:ALA:HA | 8 | 0.18 |
| (1,2124) | 1:123:A:ILE:HD12 | 1:101:A:ALA:HA | 8 | 0.18 |
| (1,2124) | 1:123:A:ILE:HD13 | 1:101:A:ALA:HA | 8 | 0.18 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 3 | 0.18 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 3 | 0.18 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 3 | 0.18 |
| (1,2047) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 1 | 0.18 |
| (1,2047) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 1 | 0.18 |
| (1,2047) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 1 | 0.18 |
| (1,1946) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HB3 | 8 | 0.18 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 8 | 0.18 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 8 | 0.18 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 8 | 0.18 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG21 | 7 | 0.18 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG22 | 7 | 0.18 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG23 | 7 | 0.18 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 5 | 0.18 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 6 | 0.18 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 7 | 0.18 |
| (1,1638) | 1:118:A:ILE:H | 1:100:A:SER:HB2 | 4 | 0.18 |
| (1,1611) | 1:98:A:THR:HA | 1:98:A:THR:HB | 3 | 0.18 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 1 | 0.18 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 2 | 0.18 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 4 | 0.18 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 4 | 0.18 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 4 | 0.18 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 2 | 0.18 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 5 | 0.18 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 10 | 0.18 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 4 | 0.18 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 9 | 0.18 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 8 | 0.18 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 4 | 0.18 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 4 | 0.18 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 4 | 0.18 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 6 | 0.18 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 6 | 0.18 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 6 | 0.18 |
| (1,1138) | 1:79:A:VAL:HG11 | 1:87:A:ASN:HB3 | 8 | 0.18 |
| (1,1138) | 1:79:A:VAL:HG12 | 1:87:A:ASN:HB3 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1138) | 1:79:A:VAL:HG13 | 1:87:A:ASN:HB3 | 8 | 0.18 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 6 | 0.18 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 2 | 0.18 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 3 | 0.18 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 5 | 0.18 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 8 | 0.18 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 10 | 0.18 |
| (1,918) | 1:60:A:LYS:HB2 | 1:59:A:LEU:HA | 1 | 0.18 |
| (1,900) | 1:57:A:ASP:HA | 1:57:A:ASP:HB3 | 10 | 0.18 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 2 | 0.18 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 9 | 0.18 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 10 | 0.18 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 10 | 0.18 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 10 | 0.18 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 10 | 0.18 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 10 | 0.18 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 10 | 0.18 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 2 | 0.18 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 4 | 0.18 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 4 | 0.18 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 4 | 0.18 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG21 | 3 | 0.18 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG22 | 3 | 0.18 |
| (1,704) | 1:44:A:ASP:H | 1:43:A:ILE:HG23 | 3 | 0.18 |
| (1,619) | 1:42:A:VAL:HG11 | 1:41:A:GLU:HA | 5 | 0.18 |
| (1,619) | 1:42:A:VAL:HG12 | 1:41:A:GLU:HA | 5 | 0.18 |
| (1,619) | 1:42:A:VAL:HG13 | 1:41:A:GLU:HA | 5 | 0.18 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 5 | 0.18 |
| (1,461) | 1:59:A:LEU:HD11 | 1:28:A:LEU:HG | 10 | 0.18 |
| (1,461) | 1:59:A:LEU:HD12 | 1:28:A:LEU:HG | 10 | 0.18 |
| (1,461) | 1:59:A:LEU:HD13 | 1:28:A:LEU:HG | 10 | 0.18 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 10 | 0.18 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 10 | 0.18 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 10 | 0.18 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 1 | 0.18 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 1 | 0.18 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 1 | 0.18 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 6 | 0.18 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 6 | 0.18 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 6 | 0.18 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 4 | 0.18 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 4 | 0.18 |
| (1,248) | 1:19:A:ILE:HD11 | 1:14:A:TRP:HZ3 | 4 | 0.18 |
| (1,248) | 1:19:A:ILE:HD12 | 1:14:A:TRP:HZ3 | 4 | 0.18 |
| (1,248) | 1:19:A:ILE:HD13 | 1:14:A:TRP:HZ3 | 4 | 0.18 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 1 | 0.18 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 1 | 0.18 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 1 | 0.18 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 4 | 0.18 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 4 | 0.18 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 4 | 0.18 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 4 | 0.18 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 8 | 0.18 |
| (3,1174) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD2 | 2 | 0.17 |
| (3,1137) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 1 | 0.17 |
| (3,1128) | 1:75:A:LYS:HG2 | 1:72:A:ALA:H | 2 | 0.17 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG21 | 2 | 0.17 |
| (3,1097) | 1:82:A:GLY:H | 1:11:A:THR:HG23 | 4 | 0.17 |
| (3,1057) | 1:8:A:THR:HB | 1:8:A:THR:HG22 | 4 | 0.17 |
| (3,1034) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 10 | 0.17 |
| (3,988) | 1:96:A:GLU:HA | 1:99:A:PHE:H | 10 | 0.17 |
| (3,854) | 1:104:A:VAL:HA | 1:103:A:ILE:HB | 3 | 0.17 |
| (3,817) | 1:84:A:TYR:HA | 1:85:A:ARG:H | 5 | 0.17 |
| (3,772) | 1:106:A:GLU:HG3 | 1:90:A:THR:H | 10 | 0.17 |
| (3,690) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 1 | 0.17 |
| (3,690) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 4 | 0.17 |
| (3,644) | 1:3:A:GLU:HA | 1:4:A:GLU:H | 7 | 0.17 |
| (3,615) | 1:26:A:LYS:HE3 | 1:30:A:GLU:HA | 10 | 0.17 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD12 | 7 | 0.17 |
| (3,545) | 1:49:A:VAL:HG12 | 1:49:A:VAL:HA | 1 | 0.17 |
| (3,545) | 1:49:A:VAL:HG13 | 1:49:A:VAL:HA | 7 | 0.17 |
| (3,523) | 1:20:A:ILE:HG22 | 1:127:A:ALA:HA | 7 | 0.17 |
| (3,523) | 1:20:A:ILE:HG22 | 1:127:A:ALA:HA | 10 | 0.17 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 3 | 0.17 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 8 | 0.17 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 9 | 0.17 |
| (3,440) | 1:103:A:ILE:H | 1:117:A:GLY:H | 10 | 0.17 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 3 | 0.17 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 4 | 0.17 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 9 | 0.17 |
| (3,353) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HB3 | 1 | 0.17 |
| (3,353) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HB3 | 8 | 0.17 |
| (3,332) | 1:43:A:ILE:HG22 | 1:43:A:ILE:HG13 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,264) | 1:77:A:ILE:H | 1:91:A:LEU:H | 4 | 0.17 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD11 | 2 | 0.17 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 3 | 0.17 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 5 | 0.17 |
| (3,153) | 1:91:A:LEU:HD11 | 1:102:A:THR:H | 8 | 0.17 |
| (2,361) | 1:84:A:TYR:HB2 | 1:103:A:ILE:HG13 | 9 | 0.17 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG11 | 9 | 0.17 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG12 | 9 | 0.17 |
| (2,357) | 1:113:A:ARG:HA | 1:115:A:VAL:HG13 | 9 | 0.17 |
| (1,3866) | 1:120:A:TYR:HE1 | 1:99:A:PHE:H | 2 | 0.17 |
| (1,3866) | 1:120:A:TYR:HE2 | 1:99:A:PHE:H | 2 | 0.17 |
| (1,3752) | 1:34:A:LYS:HG2 | 1:33:A:HIS:HE1 | 3 | 0.17 |
| (1,3696) | 1:68:A:THR:H | 1:14:A:TRP:HZ2 | 4 | 0.17 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 8 | 0.17 |
| (1,3641) | 1:11:A:THR:H | 1:81:A:ASN:HD21 | 1 | 0.17 |
| (1,3595) | 1:95:A:ASN:HD22 | 1:95:A:ASN:H | 2 | 0.17 |
| (1,3470) | 1:16:A:GLN:HB2 | 1:16:A:GLN:HE21 | 1 | 0.17 |
| (1,3468) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HE21 | 9 | 0.17 |
| (1,3468) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HE21 | 9 | 0.17 |
| (1,3468) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HE21 | 9 | 0.17 |
| (1,3434) | 1:63:A:GLN:HE22 | 1:14:A:TRP:HE1 | 4 | 0.17 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 7 | 0.17 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 7 | 0.17 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 7 | 0.17 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 7 | 0.17 |
| (1,3243) | 1:30:A:GLU:HB3 | 1:33:A:HIS:H | 4 | 0.17 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 2 | 0.17 |
| (1,3115) | 1:45:A:LYS:HB2 | 1:46:A:TYR:H | 9 | 0.17 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 8 | 0.17 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB3 | 8 | 0.17 |
| (1,2880) | 1:75:A:LYS:HB3 | 1:72:A:ALA:H | 8 | 0.17 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 3 | 0.17 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 5 | 0.17 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 7 | 0.17 |
| (1,2831) | 1:78:A:LEU:H | 1:123:A:ILE:HB | 10 | 0.17 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 3 | 0.17 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 5 | 0.17 |
| (1,2767) | 1:84:A:TYR:HB3 | 1:84:A:TYR:H | 2 | 0.17 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 2 | 0.17 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 2 | 0.17 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 2 | 0.17 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 2 | 0.17 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 10 | 0.17 |
| (1,2621) | 1:97:A:LYS:H | 1:97:A:LYS:HD2 | 6 | 0.17 |
| (1,2621) | 1:97:A:LYS:H | 1:97:A:LYS:HD2 | 7 | 0.17 |
| (1,2610) | 1:95:A:ASN:HB2 | 1:98:A:THR:H | 4 | 0.17 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 9 | 0.17 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 2 | 0.17 |
| (1,2571) | 1:117:A:GLY:HA2 | 1:101:A:ALA:H | 7 | 0.17 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 10 | 0.17 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 4 | 0.17 |
| (1,2480) | 1:111:A:LYS:HE3 | 1:111:A:LYS:H | 8 | 0.17 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 9 | 0.17 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 1 | 0.17 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 1 | 0.17 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 1 | 0.17 |
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 1 | 0.17 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 9 | 0.17 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 6 | 0.17 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 7 | 0.17 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 6 | 0.17 |
| (1,2291) | 1:68:A:THR:HA | 1:19:A:ILE:HD11 | 2 | 0.17 |
| (1,2291) | 1:68:A:THR:HA | 1:19:A:ILE:HD12 | 2 | 0.17 |
| (1,2291) | 1:68:A:THR:HA | 1:19:A:ILE:HD13 | 2 | 0.17 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG11 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG12 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG13 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG11 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG12 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG13 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG11 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG12 | 4 | 0.17 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG13 | 4 | 0.17 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 10 | 0.17 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 10 | 0.17 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 10 | 0.17 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG21 | 1 | 0.17 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 1 | 0.17 |
| (1,2242) | 1:94:A:ILE:HB | 1:70:A:ILE:HG23 | 1 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 7 | 0.17 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 7 | 0.17 |
| (1,2239) | 1:10:A:ARG:HG2 | 1:82:A:GLY:HA3 | 8 | 0.17 |
| (1,2221) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HA | 3 | 0.17 |
| (1,2221) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HA | 3 | 0.17 |
| (1,2221) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 3 | 0.17 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 8 | 0.17 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 8 | 0.17 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 8 | 0.17 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 8 | 0.17 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 8 | 0.17 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 8 | 0.17 |
| (1,2205) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 2 | 0.17 |
| (1,2205) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 2 | 0.17 |
| (1,2205) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 2 | 0.17 |
| (1,2051) | 1:124:A:SER:HB2 | 1:68:A:THR:HB | 3 | 0.17 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG21 | 7 | 0.17 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG22 | 7 | 0.17 |
| (1,2032) | 1:78:A:LEU:H | 1:123:A:ILE:HG23 | 7 | 0.17 |
| (1,1997) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 5 | 0.17 |
| (1,1971) | 1:119:A:GLN:HA | 1:101:A:ALA:H | 4 | 0.17 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 3 | 0.17 |
| (1,1947) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HA | 2 | 0.17 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 7 | 0.17 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 7 | 0.17 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 7 | 0.17 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 10 | 0.17 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 10 | 0.17 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 10 | 0.17 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 3 | 0.17 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 3 | 0.17 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 3 | 0.17 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 7 | 0.17 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 7 | 0.17 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 7 | 0.17 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG21 | 6 | 0.17 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG22 | 6 | 0.17 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG23 | 6 | 0.17 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 5 | 0.17 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 5 | 0.17 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 4 | 0.17 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 6 | 0.17 |
| (1,1610) | 1:98:A:THR:H | 1:98:A:THR:HA | 6 | 0.17 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 7 | 0.17 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 1 | 0.17 |
| (1,1459) | 1:87:A:ASN:H | 1:87:A:ASN:HB3 | 9 | 0.17 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 7 | 0.17 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 7 | 0.17 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 7 | 0.17 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 1 | 0.17 |
| (1,1206) | 1:71:A:PRO:HD2 | 1:70:A:ILE:HG21 | 10 | 0.17 |
| (1,1206) | 1:71:A:PRO:HD2 | 1:70:A:ILE:HG22 | 10 | 0.17 |
| (1,1206) | 1:71:A:PRO:HD2 | 1:70:A:ILE:HG23 | 10 | 0.17 |
| (1,1138) | 1:79:A:VAL:HG11 | 1:87:A:ASN:HB3 | 6 | 0.17 |
| (1,1138) | 1:79:A:VAL:HG12 | 1:87:A:ASN:HB3 | 6 | 0.17 |
| (1,1138) | 1:79:A:VAL:HG13 | 1:87:A:ASN:HB3 | 6 | 0.17 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 7 | 0.17 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 8 | 0.17 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 5 | 0.17 |
| (1,922) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 3 | 0.17 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG21 | 3 | 0.17 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG22 | 3 | 0.17 |
| (1,881) | 1:54:A:ASP:HA | 1:53:A:ILE:HG23 | 3 | 0.17 |
| (1,849) | 1:37:A:ALA:HA | 1:53:A:ILE:HB | 5 | 0.17 |
| (1,818) | 1:51:A:LYS:HG2 | 1:56:A:GLY:HA3 | 8 | 0.17 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 1 | 0.17 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 4 | 0.17 |
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 4 | 0.17 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 4 | 0.17 |
| (1,683) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HA | 4 | 0.17 |
| (1,683) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HA | 4 | 0.17 |
| (1,683) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HA | 4 | 0.17 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG21 | 4 | 0.17 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG22 | 4 | 0.17 |
| (1,662) | 1:45:A:LYS:HA | 1:42:A:VAL:HG23 | 4 | 0.17 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 2 | 0.17 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 2 | 0.17 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 2 | 0.17 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 3 | 0.17 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 4 | 0.17 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 4 | 0.17 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 4 | 0.17 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 4 | 0.17 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 4 | 0.17 |
| (1,440) | 1:111:A:LYS:HD2 | 1:107:A:THR:HA | 5 | 0.17 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD11 | 7 | 0.17 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD12 | 7 | 0.17 |
| (1,353) | 1:35:A:LYS:H | 1:23:A:ILE:HD13 | 7 | 0.17 |
| (1,154) | 1:16:A:GLN:HA | 1:16:A:GLN:HB3 | 5 | 0.17 |
| (1,154) | 1:16:A:GLN:HA | 1:16:A:GLN:HB3 | 8 | 0.17 |
| (1,154) | 1:16:A:GLN:HA | 1:16:A:GLN:HB3 | 10 | 0.17 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 7 | 0.17 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 7 | 0.17 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 7 | 0.17 |
| (1,70) | 1:11:A:THR:HA | 1:11:A:THR:HB | 4 | 0.17 |
| (1,1) | 1:107:A:THR:HB | 1:108:A:GLY:H | 1 | 0.17 |
| (3,1182) | 1:98:A:THR:HG22 | 1:98:A:THR:HA | 10 | 0.16 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG21 | 3 | 0.16 |
| (3,1042) | 1:19:A:ILE:HA | 1:127:A:ALA:HA | 8 | 0.16 |
| (3,1034) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 6 | 0.16 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG21 | 9 | 0.16 |
| (3,895) | 1:126:A:LEU:HD23 | 1:89:A:GLY:H | 6 | 0.16 |
| (3,890) | 1:78:A:LEU:HA | 1:124:A:SER:H | 2 | 0.16 |
| (3,854) | 1:104:A:VAL:HA | 1:103:A:ILE:HB | 5 | 0.16 |
| (3,838) | 1:52:A:MET:H | 1:59:A:LEU:H | 2 | 0.16 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 2 | 0.16 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 10 | 0.16 |
| (3,816) | 1:77:A:ILE:H | 1:91:A:LEU:H | 1 | 0.16 |
| (3,799) | 1:48:A:ALA:H | 1:60:A:LYS:HD3 | 3 | 0.16 |
| (3,735) | 1:115:A:VAL:HG12 | 1:103:A:ILE:HD12 | 7 | 0.16 |
| (3,732) | 1:48:A:ALA:HB3 | 1:43:A:ILE:H | 8 | 0.16 |
| (3,690) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 2 | 0.16 |
| (3,690) | 1:58:A:LYS:HG2 | 1:58:A:LYS:HE2 | 7 | 0.16 |
| (3,690) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HG2 | 9 | 0.16 |
| (3,690) | 1:58:A:LYS:HG2 | 1:58:A:LYS:HE2 | 10 | 0.16 |
| (3,655) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HD3 | 3 | 0.16 |
| (3,655) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HD3 | 7 | 0.16 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 3 | 0.16 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD11 | 2 | 0.16 |
| (3,487) | 1:6:A:LYS:HG2 | 1:6:A:LYS:HE2 | 1 | 0.16 |
| (3,440) | 1:103:A:ILE:H | 1:117:A:GLY:H | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,423) | 1:61:A:LEU:HD12 | 1:25:A:THR:H | 6 | 0.16 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 10 | 0.16 |
| (3,353) | 1:61:A:LEU:HD21 | 1:61:A:LEU:HB3 | 2 | 0.16 |
| (3,353) | 1:61:A:LEU:HD23 | 1:61:A:LEU:HB3 | 4 | 0.16 |
| (3,353) | 1:61:A:LEU:HD21 | 1:61:A:LEU:HB3 | 5 | 0.16 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD13 | 2 | 0.16 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD11 | 7 | 0.16 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD12 | 10 | 0.16 |
| (3,304) | 1:94:A:ILE:HB | 1:70:A:ILE:HG22 | 5 | 0.16 |
| (3,303) | 1:102:A:THR:HA | 1:103:A:ILE:HD13 | 5 | 0.16 |
| (3,268) | 1:125:A:LYS:HE2 | 1:125:A:LYS:HE3 | 1 | 0.16 |
| (3,268) | 1:125:A:LYS:HE2 | 1:125:A:LYS:HE3 | 2 | 0.16 |
| (3,268) | 1:125:A:LYS:HE2 | 1:125:A:LYS:HE3 | 3 | 0.16 |
| (3,268) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HE2 | 4 | 0.16 |
| (3,268) | 1:125:A:LYS:HE2 | 1:125:A:LYS:HE3 | 5 | 0.16 |
| (3,268) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HE2 | 6 | 0.16 |
| (3,268) | 1:51:A:LYS:HE3 | 1:51:A:LYS:HE2 | 7 | 0.16 |
| (3,268) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HE2 | 8 | 0.16 |
| (3,268) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HE2 | 9 | 0.16 |
| (3,268) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HE2 | 10 | 0.16 |
| (3,165) | 1:79:A:VAL:HG12 | 1:88:A:GLU:HA | 1 | 0.16 |
| (3,165) | 1:79:A:VAL:HG11 | 1:88:A:GLU:HA | 10 | 0.16 |
| (3,108) | 1:45:A:LYS:HG3 | 1:45:A:LYS:HE3 | 2 | 0.16 |
| (3,21) | 1:126:A:LEU:HD21 | 1:88:A:GLU:HG2 | 2 | 0.16 |
| (2,574) | 1:39:A:VAL:H | 1:20:A:ILE:HG12 | 7 | 0.16 |
| (2,230) | 1:110:A:LEU:HD21 | 1:84:A:TYR:H | 10 | 0.16 |
| (2,230) | 1:110:A:LEU:HD22 | 1:84:A:TYR:H | 10 | 0.16 |
| (2,230) | 1:110:A:LEU:HD23 | 1:84:A:TYR:H | 10 | 0.16 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 9 | 0.16 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 9 | 0.16 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD11 | 1 | 0.16 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD12 | 1 | 0.16 |
| (1,3849) | 1:84:A:TYR:HE1 | 1:105:A:ILE:HD13 | 1 | 0.16 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD11 | 1 | 0.16 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD12 | 1 | 0.16 |
| (1,3849) | 1:84:A:TYR:HE2 | 1:105:A:ILE:HD13 | 1 | 0.16 |
| (1,3728) | 1:97:A:LYS:H | 1:95:A:ASN:HD21 | 5 | 0.16 |
| (1,3697) | 1:68:A:THR:H | 1:14:A:TRP:HE1 | 1 | 0.16 |
| (1,3656) | 1:32:A:TYR:HB2 | 1:27:A:LYS:H | 5 | 0.16 |
| (1,3591) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD21 | 7 | 0.16 |
| (1,3591) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD21 | 7 | 0.16 |
| (1,3591) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD21 | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3591) | 1:98:A:THR:HG21 | 1:95:A:ASN:HD21 | 8 | 0.16 |
| (1,3591) | 1:98:A:THR:HG22 | 1:95:A:ASN:HD21 | 8 | 0.16 |
| (1,3591) | 1:98:A:THR:HG23 | 1:95:A:ASN:HD21 | 8 | 0.16 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 4 | 0.16 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 4 | 0.16 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 4 | 0.16 |
| (1,3542) | 1:64:A:THR:H | 1:14:A:TRP:HE1 | 6 | 0.16 |
| (1,3537) | 1:46:A:TYR:HE1 | 1:63:A:GLN:HE21 | 3 | 0.16 |
| (1,3537) | 1:46:A:TYR:HE2 | 1:63:A:GLN:HE21 | 3 | 0.16 |
| (1,3537) | 1:46:A:TYR:HE1 | 1:63:A:GLN:HE21 | 9 | 0.16 |
| (1,3537) | 1:46:A:TYR:HE2 | 1:63:A:GLN:HE21 | 9 | 0.16 |
| (1,3459) | 1:80:A:LEU:HD21 | 1:16:A:GLN:HE22 | 10 | 0.16 |
| (1,3459) | 1:80:A:LEU:HD22 | 1:16:A:GLN:HE22 | 10 | 0.16 |
| (1,3459) | 1:80:A:LEU:HD23 | 1:16:A:GLN:HE22 | 10 | 0.16 |
| (1,3397) | 1:10:A:ARG:HB3 | 1:11:A:THR:H | 9 | 0.16 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 2 | 0.16 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 2 | 0.16 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 2 | 0.16 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 3 | 0.16 |
| (1,3113) | 1:44:A:ASP:HB2 | 1:46:A:TYR:H | 9 | 0.16 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 5 | 0.16 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 5 | 0.16 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 5 | 0.16 |
| (1,3021) | 1:51:A:LYS:HD2 | 1:57:A:ASP:H | 1 | 0.16 |
| (1,2976) | 1:63:A:GLN:H | 1:14:A:TRP:HE1 | 8 | 0.16 |
| (1,2967) | 1:46:A:TYR:HB2 | 1:63:A:GLN:H | 5 | 0.16 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 2 | 0.16 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 4 | 0.16 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 9 | 0.16 |
| (1,2788) | 1:81:A:ASN:H | 1:84:A:TYR:H | 7 | 0.16 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 4 | 0.16 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 4 | 0.16 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 4 | 0.16 |
| (1,2641) | 1:95:A:ASN:HD21 | 1:95:A:ASN:H | 1 | 0.16 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 5 | 0.16 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 8 | 0.16 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 4 | 0.16 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 7 | 0.16 |
| (1,2509) | 1:107:A:THR:H | 1:88:A:GLU:H | 9 | 0.16 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG21 | 9 | 0.16 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG22 | 9 | 0.16 |
| (1,2468) | 1:113:A:ARG:H | 1:105:A:ILE:HG23 | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 7 | 0.16 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 5 | 0.16 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 7 | 0.16 |
| (1,2429) | 1:93:A:SER:H | 1:91:A:LEU:HG | 8 | 0.16 |
| (1,2411) | 1:118:A:ILE:H | 1:101:A:ALA:HA | 7 | 0.16 |
| (1,2401) | 1:122:A:ASP:HB3 | 1:119:A:GLN:H | 6 | 0.16 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 4 | 0.16 |
| (1,2316) | 1:127:A:ALA:H | 1:19:A:ILE:HB | 3 | 0.16 |
| (1,2304) | 1:104:A:VAL:HG21 | 1:114:A:ARG:HB3 | 7 | 0.16 |
| (1,2304) | 1:104:A:VAL:HG22 | 1:114:A:ARG:HB3 | 7 | 0.16 |
| (1,2304) | 1:104:A:VAL:HG23 | 1:114:A:ARG:HB3 | 7 | 0.16 |
| (1,2277) | 1:21:A:VAL:HG21 | 1:66:A:LEU:HA | 8 | 0.16 |
| (1,2277) | 1:21:A:VAL:HG22 | 1:66:A:LEU:HA | 8 | 0.16 |
| (1,2277) | 1:21:A:VAL:HG23 | 1:66:A:LEU:HA | 8 | 0.16 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 10 | 0.16 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 10 | 0.16 |
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 10 | 0.16 |
| (1,2196) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 3 | 0.16 |
| (1,2157) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB3 | 4 | 0.16 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 1 | 0.16 |
| (1,1997) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 7 | 0.16 |
| (1,1997) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 10 | 0.16 |
| (1,1971) | 1:119:A:GLN:HA | 1:101:A:ALA:H | 8 | 0.16 |
| (1,1966) | 1:118:A:ILE:HG21 | 1:122:A:ASP:H | 3 | 0.16 |
| (1,1966) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 3 | 0.16 |
| (1,1966) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 3 | 0.16 |
| (1,1959) | 1:118:A:ILE:HD11 | 1:122:A:ASP:HB2 | 4 | 0.16 |
| (1,1959) | 1:118:A:ILE:HD12 | 1:122:A:ASP:HB2 | 4 | 0.16 |
| (1,1959) | 1:118:A:ILE:HD13 | 1:122:A:ASP:HB2 | 4 | 0.16 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 3 | 0.16 |
| (1,1760) | 1:105:A:ILE:HG21 | 1:111:A:LYS:H | 2 | 0.16 |
| (1,1760) | 1:105:A:ILE:HG22 | 1:111:A:LYS:H | 2 | 0.16 |
| (1,1760) | 1:105:A:ILE:HG23 | 1:111:A:LYS:H | 2 | 0.16 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD11 | 4 | 0.16 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD12 | 4 | 0.16 |
| (1,1742) | 1:84:A:TYR:HB2 | 1:105:A:ILE:HD13 | 4 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 8 | 0.16 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 8 | 0.16 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 9 | 0.16 |
| (1,1678) | 1:102:A:THR:HG21 | 1:103:A:ILE:HA | 9 | 0.16 |
| (1,1678) | 1:102:A:THR:HG22 | 1:103:A:ILE:HA | 9 | 0.16 |
| (1,1678) | 1:102:A:THR:HG23 | 1:103:A:ILE:HA | 9 | 0.16 |
| (1,1667) | 1:102:A:THR:HA | 1:116:A:GLU:HG2 | 9 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 2 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 2 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 2 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 7 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 7 | 0.16 |
| (1,1655) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 7 | 0.16 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 5 | 0.16 |
| (1,1555) | 1:93:A:SER:HA | 1:73:A:PRO:HG2 | 1 | 0.16 |
| (1,1441) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 9 | 0.16 |
| (1,1352) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA2 | 10 | 0.16 |
| (1,1352) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA2 | 10 | 0.16 |
| (1,1352) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA2 | 10 | 0.16 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG21 | 2 | 0.16 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG22 | 2 | 0.16 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG23 | 2 | 0.16 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG21 | 5 | 0.16 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG22 | 5 | 0.16 |
| (1,1321) | 1:71:A:PRO:HG3 | 1:77:A:ILE:HG23 | 5 | 0.16 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 1 | 0.16 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 2 | 0.16 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 5 | 0.16 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 5 | 0.16 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 5 | 0.16 |
| (1,1138) | 1:79:A:VAL:HG11 | 1:87:A:ASN:HB3 | 1 | 0.16 |
| (1,1138) | 1:79:A:VAL:HG12 | 1:87:A:ASN:HB3 | 1 | 0.16 |
| (1,1138) | 1:79:A:VAL:HG13 | 1:87:A:ASN:HB3 | 1 | 0.16 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 1 | 0.16 |
| (1,1036) | 1:64:A:THR:HA | 1:64:A:THR:HB | 9 | 0.16 |
| (1,1021) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 3 | 0.16 |
| (1,1021) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 3 | 0.16 |
| (1,1021) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 3 | 0.16 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 6 | 0.16 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 2 | 0.16 |
| (1,893) | 1:51:A:LYS:HG2 | 1:56:A:GLY:HA3 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 2 | 0.16 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 5 | 0.16 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 8 | 0.16 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 10 | 0.16 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 3 | 0.16 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 8 | 0.16 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 1 | 0.16 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 1 | 0.16 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 1 | 0.16 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 7 | 0.16 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 7 | 0.16 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 7 | 0.16 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 8 | 0.16 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 8 | 0.16 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 8 | 0.16 |
| (1,717) | 1:45:A:LYS:HA | 1:45:A:LYS:HG3 | 4 | 0.16 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 6 | 0.16 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 6 | 0.16 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 6 | 0.16 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 1 | 0.16 |
| (1,479) | 1:31:A:LYS:HA | 1:32:A:TYR:H | 5 | 0.16 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 5 | 0.16 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 5 | 0.16 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 5 | 0.16 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 5 | 0.16 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 5 | 0.16 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 5 | 0.16 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 10 | 0.16 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 10 | 0.16 |
| (1,384) | 1:24:A:ILE:HD11 | 1:65:A:HIS:H | 6 | 0.16 |
| (1,384) | 1:24:A:ILE:HD12 | 1:65:A:HIS:H | 6 | 0.16 |
| (1,384) | 1:24:A:ILE:HD13 | 1:65:A:HIS:H | 6 | 0.16 |
| (1,375) | 1:23:A:ILE:HG21 | 1:66:A:LEU:HA | 9 | 0.16 |
| (1,375) | 1:23:A:ILE:HG22 | 1:66:A:LEU:HA | 9 | 0.16 |
| (1,375) | 1:23:A:ILE:HG23 | 1:66:A:LEU:HA | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 1 | 0.16 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 2 | 0.16 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 9 | 0.16 |
| (1,154) | 1:16:A:GLN:HA | 1:16:A:GLN:HB3 | 7 | 0.16 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 1 | 0.16 |
| (1,70) | 1:11:A:THR:HA | 1:11:A:THR:HB | 3 | 0.16 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 6 | 0.16 |
| (3,1221) | 1:61:A:LEU:HD11 | 1:59:A:LEU:HD13 | 10 | 0.15 |
| (3,1173) | 1:84:A:TYR:HE2 | 1:110:A:LEU:HB2 | 10 | 0.15 |
| (3,1164) | 1:26:A:LYS:HG3 | 1:29:A:GLY:H | 3 | 0.15 |
| (3,1101) | 1:123:A:ILE:H | 1:121:A:GLU:HG3 | 3 | 0.15 |
| (3,1074) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 4 | 0.15 |
| (3,1068) | 1:126:A:LEU:H | 1:76:A:ARG:HB2 | 2 | 0.15 |
| (3,1057) | 1:8:A:THR:HB | 1:8:A:THR:HG21 | 6 | 0.15 |
| (3,993) | 1:58:A:LYS:HG3 | 1:50:A:VAL:H | 6 | 0.15 |
| (3,973) | 1:20:A:ILE:HG21 | 1:21:A:VAL:H | 1 | 0.15 |
| (3,928) | 1:120:A:TYR:HA | 1:123:A:ILE:HG22 | 2 | 0.15 |
| (3,867) | 1:17:A:PRO:HB3 | 1:18:A:GLU:H | 9 | 0.15 |
| (3,838) | 1:52:A:MET:H | 1:59:A:LEU:H | 4 | 0.15 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG23 | 5 | 0.15 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG22 | 6 | 0.15 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG23 | 7 | 0.15 |
| (3,655) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HG | 5 | 0.15 |
| (3,655) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HG | 8 | 0.15 |
| (3,655) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HD3 | 9 | 0.15 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 8 | 0.15 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 6 | 0.15 |
| (3,552) | 1:32:A:TYR:HE1 | 1:57:A:ASP:HB3 | 1 | 0.15 |
| (3,545) | 1:49:A:VAL:HG12 | 1:49:A:VAL:HA | 6 | 0.15 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 9 | 0.15 |
| (3,423) | 1:61:A:LEU:HD12 | 1:25:A:THR:H | 10 | 0.15 |
| (3,409) | 1:96:A:GLU:HB2 | 1:96:A:GLU:HG3 | 2 | 0.15 |
| (3,396) | 1:118:A:ILE:HG23 | 1:121:A:GLU:HA | 5 | 0.15 |
| (3,381) | 1:45:A:LYS:H | 1:44:A:ASP:HB3 | 1 | 0.15 |
| (3,379) | 1:45:A:LYS:HA | 1:13:A:TYR:HD2 | 3 | 0.15 |
| (3,366) | 1:42:A:VAL:HG22 | 1:16:A:GLN:HG2 | 10 | 0.15 |
| (3,332) | 1:43:A:ILE:HG21 | 1:43:A:ILE:HG13 | 8 | 0.15 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD12 | 1 | 0.15 |
| (3,321) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HG | 3 | 0.15 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD13 | 4 | 0.15 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD12 | 5 | 0.15 |
| (3,321) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HG | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD13 | 8 | 0.15 |
| (3,321) | 1:118:A:ILE:HG12 | 1:118:A:ILE:HD11 | 9 | 0.15 |
| (3,310) | 1:111:A:LYS:HD3 | 1:111:A:LYS:HG3 | 2 | 0.15 |
| (3,303) | 1:102:A:THR:HA | 1:103:A:ILE:HD13 | 2 | 0.15 |
| (3,180) | 1:65:A:HIS:H | 1:62:A:ASP:HB3 | 10 | 0.15 |
| (3,148) | 1:73:A:PRO:HG2 | 1:93:A:SER:HB3 | 8 | 0.15 |
| (3,140) | 1:78:A:LEU:HD21 | 1:88:A:GLU:HG3 | 9 | 0.15 |
| (3,129) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HB | 4 | 0.15 |
| (3,128) | 1:77:A:ILE:HD12 | 1:123:A:ILE:HG22 | 5 | 0.15 |
| (3,85) | 1:39:A:VAL:HG22 | 1:50:A:VAL:HA | 2 | 0.15 |
| (3,85) | 1:39:A:VAL:HG21 | 1:50:A:VAL:HA | 7 | 0.15 |
| (3,60) | 1:53:A:ILE:HG22 | 1:53:A:ILE:HB | 2 | 0.15 |
| (3,60) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 8 | 0.15 |
| (2,407) | 1:42:A:VAL:HG11 | 1:44:A:ASP:HA | 1 | 0.15 |
| (2,407) | 1:42:A:VAL:HG12 | 1:44:A:ASP:HA | 1 | 0.15 |
| (2,407) | 1:42:A:VAL:HG13 | 1:44:A:ASP:HA | 1 | 0.15 |
| (2,356) | 1:115:A:VAL:HG11 | 1:84:A:TYR:HA | 9 | 0.15 |
| (2,356) | 1:115:A:VAL:HG12 | 1:84:A:TYR:HA | 9 | 0.15 |
| (2,356) | 1:115:A:VAL:HG13 | 1:84:A:TYR:HA | 9 | 0.15 |
| (1,3771) | 1:13:A:TYR:HA | 1:46:A:TYR:HD1 | 10 | 0.15 |
| (1,3771) | 1:13:A:TYR:HA | 1:46:A:TYR:HD2 | 10 | 0.15 |
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 10 | 0.15 |
| (1,3737) | 1:5:A:LYS:H | 1:3:A:GLU:H | 2 | 0.15 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 8 | 0.15 |
| (1,3705) | 1:75:A:LYS:H | 1:91:A:LEU:HA | 2 | 0.15 |
| (1,3705) | 1:75:A:LYS:H | 1:91:A:LEU:HA | 5 | 0.15 |
| (1,3700) | 1:72:A:ALA:H | 1:71:A:PRO:HB2 | 2 | 0.15 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 2 | 0.15 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 5 | 0.15 |
| (1,3656) | 1:32:A:TYR:HB2 | 1:27:A:LYS:H | 7 | 0.15 |
| (1,3643) | 1:13:A:TYR:H | 1:63:A:GLN:HE21 | 6 | 0.15 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 1 | 0.15 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 2 | 0.15 |
| (1,3587) | 1:95:A:ASN:HA | 1:95:A:ASN:HD21 | 4 | 0.15 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 5 | 0.15 |
| (1,3471) | 1:42:A:VAL:HG11 | 1:16:A:GLN:HE21 | 3 | 0.15 |
| (1,3471) | 1:42:A:VAL:HG12 | 1:16:A:GLN:HE21 | 3 | 0.15 |
| (1,3471) | 1:42:A:VAL:HG13 | 1:16:A:GLN:HE21 | 3 | 0.15 |
| (1,3403) | 1:10:A:ARG:HD2 | 1:10:A:ARG:H | 4 | 0.15 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD11 | 9 | 0.15 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD12 | 9 | 0.15 |
| (1,3278) | 1:28:A:LEU:H | 1:28:A:LEU:HD13 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 7 | 0.15 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 7 | 0.15 |
| (1,3122) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 7 | 0.15 |
| (1,3015) | 1:32:A:TYR:HE1 | 1:57:A:ASP:H | 10 | 0.15 |
| (1,3015) | 1:32:A:TYR:HE2 | 1:57:A:ASP:H | 10 | 0.15 |
| (1,3011) | 1:58:A:LYS:H | 1:57:A:ASP:HB3 | 2 | 0.15 |
| (1,2970) | 1:63:A:GLN:H | 1:64:A:THR:HG21 | 1 | 0.15 |
| (1,2970) | 1:63:A:GLN:H | 1:64:A:THR:HG22 | 1 | 0.15 |
| (1,2970) | 1:63:A:GLN:H | 1:64:A:THR:HG23 | 1 | 0.15 |
| (1,2967) | 1:46:A:TYR:HB2 | 1:63:A:GLN:H | 9 | 0.15 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 4 | 0.15 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 9 | 0.15 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 1 | 0.15 |
| (1,2831) | 1:78:A:LEU:H | 1:123:A:ILE:HB | 1 | 0.15 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 5 | 0.15 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 1 | 0.15 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 6 | 0.15 |
| (1,2747) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 1 | 0.15 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 8 | 0.15 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 9 | 0.15 |
| (1,2636) | 1:96:A:GLU:H | 1:97:A:LYS:HD2 | 2 | 0.15 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 2 | 0.15 |
| (1,2509) | 1:107:A:THR:H | 1:88:A:GLU:H | 4 | 0.15 |
| (1,2477) | 1:110:A:LEU:HB3 | 1:111:A:LYS:H | 2 | 0.15 |
| (1,2363) | 1:70:A:ILE:HD11 | 1:121:A:GLU:H | 10 | 0.15 |
| (1,2363) | 1:70:A:ILE:HD12 | 1:121:A:GLU:H | 10 | 0.15 |
| (1,2363) | 1:70:A:ILE:HD13 | 1:121:A:GLU:H | 10 | 0.15 |
| (1,2339) | 1:77:A:ILE:HA | 1:124:A:SER:H | 5 | 0.15 |
| (1,2294) | 1:19:A:ILE:HD11 | 1:16:A:GLN:HB2 | 2 | 0.15 |
| (1,2294) | 1:19:A:ILE:HD12 | 1:16:A:GLN:HB2 | 2 | 0.15 |
| (1,2294) | 1:19:A:ILE:HD13 | 1:16:A:GLN:HB2 | 2 | 0.15 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 9 | 0.15 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 9 | 0.15 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 9 | 0.15 |
| (1,2218) | 1:102:A:THR:HB | 1:103:A:ILE:H | 5 | 0.15 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 8 | 0.15 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 8 | 0.15 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 8 | 0.15 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG21 | 8 | 0.15 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG22 | 8 | 0.15 |
| (1,2172) | 1:113:A:ARG:HB3 | 1:105:A:ILE:HG23 | 8 | 0.15 |
| (1,2157) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB3 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 9 | 0.15 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 9 | 0.15 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 9 | 0.15 |
| (1,1916) | 1:115:A:VAL:HG11 | 1:105:A:ILE:H | 5 | 0.15 |
| (1,1916) | 1:115:A:VAL:HG12 | 1:105:A:ILE:H | 5 | 0.15 |
| (1,1916) | 1:115:A:VAL:HG13 | 1:105:A:ILE:H | 5 | 0.15 |
| (1,1885) | 1:115:A:VAL:HG11 | 1:113:A:ARG:HD2 | 8 | 0.15 |
| (1,1885) | 1:115:A:VAL:HG12 | 1:113:A:ARG:HD2 | 8 | 0.15 |
| (1,1885) | 1:115:A:VAL:HG13 | 1:113:A:ARG:HD2 | 8 | 0.15 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 3 | 0.15 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 3 | 0.15 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 3 | 0.15 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG21 | 3 | 0.15 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG22 | 3 | 0.15 |
| (1,1758) | 1:110:A:LEU:H | 1:105:A:ILE:HG23 | 3 | 0.15 |
| (1,1739) | 1:84:A:TYR:HD1 | 1:105:A:ILE:HD11 | 3 | 0.15 |
| (1,1739) | 1:84:A:TYR:HD1 | 1:105:A:ILE:HD12 | 3 | 0.15 |
| (1,1739) | 1:84:A:TYR:HD1 | 1:105:A:ILE:HD13 | 3 | 0.15 |
| (1,1739) | 1:84:A:TYR:HD2 | 1:105:A:ILE:HD11 | 3 | 0.15 |
| (1,1739) | 1:84:A:TYR:HD2 | 1:105:A:ILE:HD12 | 3 | 0.15 |
| (1,1739) | 1:84:A:TYR:HD2 | 1:105:A:ILE:HD13 | 3 | 0.15 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 4 | 0.15 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 8 | 0.15 |
| (1,1680) | 1:102:A:THR:HG21 | 1:116:A:GLU:HG3 | 6 | 0.15 |
| (1,1680) | 1:102:A:THR:HG22 | 1:116:A:GLU:HG3 | 6 | 0.15 |
| (1,1680) | 1:102:A:THR:HG23 | 1:116:A:GLU:HG3 | 6 | 0.15 |
| (1,1658) | 1:102:A:THR:H | 1:101:A:ALA:HB1 | 4 | 0.15 |
| (1,1658) | 1:102:A:THR:H | 1:101:A:ALA:HB2 | 4 | 0.15 |
| (1,1658) | 1:102:A:THR:H | 1:101:A:ALA:HB3 | 4 | 0.15 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 1 | 0.15 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 8 | 0.15 |
| (1,1611) | 1:98:A:THR:HA | 1:98:A:THR:HB | 9 | 0.15 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 6 | 0.15 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 6 | 0.15 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 6 | 0.15 |
| (1,1531) | 1:92:A:GLU:HA | 1:74:A:GLY:H | 10 | 0.15 |
| (1,1492) | 1:104:A:VAL:H | 1:90:A:THR:HB | 6 | 0.15 |
| (1,1492) | 1:104:A:VAL:H | 1:90:A:THR:HB | 10 | 0.15 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 3 | 0.15 |
| (1,1386) | 1:81:A:ASN:HA | 1:81:A:ASN:HB2 | 1 | 0.15 |
| (1,1386) | 1:81:A:ASN:HA | 1:81:A:ASN:HB2 | 9 | 0.15 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 1 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 1 | 0.15 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 1 | 0.15 |
| (1,1277) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 9 | 0.15 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB1 | 5 | 0.15 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB2 | 5 | 0.15 |
| (1,1216) | 1:75:A:LYS:HG2 | 1:72:A:ALA:HB3 | 5 | 0.15 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 6 | 0.15 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 6 | 0.15 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 6 | 0.15 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 3 | 0.15 |
| (1,1104) | 1:67:A:GLU:HA | 1:67:A:GLU:HG2 | 9 | 0.15 |
| (1,1068) | 1:21:A:VAL:HB | 1:66:A:LEU:HA | 7 | 0.15 |
| (1,957) | 1:60:A:LYS:HB3 | 1:59:A:LEU:HA | 7 | 0.15 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 6 | 0.15 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 8 | 0.15 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 8 | 0.15 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 8 | 0.15 |
| (1,906) | 1:58:A:LYS:H | 1:57:A:ASP:HB2 | 2 | 0.15 |
| (1,906) | 1:58:A:LYS:H | 1:57:A:ASP:HB2 | 10 | 0.15 |
| (1,900) | 1:57:A:ASP:HA | 1:57:A:ASP:HB3 | 4 | 0.15 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 10 | 0.15 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 6 | 0.15 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 6 | 0.15 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 6 | 0.15 |
| (1,711) | 1:45:A:LYS:H | 1:44:A:ASP:HB2 | 3 | 0.15 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 3 | 0.15 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 3 | 0.15 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 3 | 0.15 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 8 | 0.15 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 8 | 0.15 |
| (1,695) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 8 | 0.15 |
| (1,683) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HA | 6 | 0.15 |
| (1,683) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HA | 6 | 0.15 |
| (1,683) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HA | 6 | 0.15 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 1 | 0.15 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 1 | 0.15 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 1 | 0.15 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG11 | 9 | 0.15 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG12 | 9 | 0.15 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG13 | 9 | 0.15 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 8 | 0.15 |
| (1,629) | 1:104:A:VAL:HB | 1:104:A:VAL:H | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 9 | 0.15 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 9 | 0.15 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 9 | 0.15 |
| (1,479) | 1:31:A:LYS:HA | 1:32:A:TYR:H | 6 | 0.15 |
| (1,455) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HB3 | 3 | 0.15 |
| (1,455) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HB3 | 3 | 0.15 |
| (1,455) | 1:28:A:LEU:HD13 | 1:28:A:LEU:HB3 | 3 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 2 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 4 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 5 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 6 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 7 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 8 | 0.15 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 8 | 0.15 |
| (1,426) | 1:91:A:LEU:HD21 | 1:102:A:THR:H | 1 | 0.15 |
| (1,426) | 1:91:A:LEU:HD22 | 1:102:A:THR:H | 1 | 0.15 |
| (1,426) | 1:91:A:LEU:HD23 | 1:102:A:THR:H | 1 | 0.15 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG21 | 6 | 0.15 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG22 | 6 | 0.15 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG23 | 6 | 0.15 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD11 | 4 | 0.15 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD12 | 4 | 0.15 |
| (1,387) | 1:65:A:HIS:HA | 1:24:A:ILE:HD13 | 4 | 0.15 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 4 | 0.15 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 4 | 0.15 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 4 | 0.15 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 4 | 0.15 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 9 | 0.15 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 9 | 0.15 |
| (3,1167) | 1:115:A:VAL:HG21 | 1:115:A:VAL:HB | 4 | 0.14 |
| (3,1167) | 1:115:A:VAL:HG22 | 1:115:A:VAL:HB | 8 | 0.14 |
| (3,1146) | 1:115:A:VAL:HA | 1:103:A:ILE:H | 1 | 0.14 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG23 | 9 | 0.14 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG23 | 10 | 0.14 |
| (3,993) | 1:61:A:LEU:HG | 1:50:A:VAL:H | 10 | 0.14 |
| (3,965) | 1:95:A:ASN:H | 1:101:A:ALA:H | 5 | 0.14 |
| (3,928) | 1:94:A:ILE:HG22 | 1:91:A:LEU:HA | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,919) | 1:27:A:LYS:HD3 | 1:65:A:HIS:HE1 | 1 | 0.14 |
| (3,900) | 1:34:A:LYS:HE3 | 1:34:A:LYS:HG3 | 7 | 0.14 |
| (3,890) | 1:68:A:THR:HB | 1:124:A:SER:H | 10 | 0.14 |
| (3,854) | 1:104:A:VAL:HA | 1:103:A:ILE:HB | 2 | 0.14 |
| (3,826) | 1:5:A:LYS:H | 1:5:A:LYS:HA | 5 | 0.14 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 1 | 0.14 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 3 | 0.14 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG22 | 4 | 0.14 |
| (3,819) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HG | 5 | 0.14 |
| (3,817) | 1:84:A:TYR:HA | 1:85:A:ARG:H | 4 | 0.14 |
| (3,655) | 1:28:A:LEU:HD22 | 1:28:A:LEU:HG | 4 | 0.14 |
| (3,655) | 1:28:A:LEU:HD23 | 1:28:A:LEU:HG | 6 | 0.14 |
| (3,633) | 1:51:A:LYS:HG3 | 1:56:A:GLY:H | 5 | 0.14 |
| (3,559) | 1:23:A:ILE:HD11 | 1:33:A:HIS:H | 6 | 0.14 |
| (3,518) | 1:96:A:GLU:HG3 | 1:97:A:LYS:HG3 | 4 | 0.14 |
| (3,487) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HB | 6 | 0.14 |
| (3,487) | 1:75:A:LYS:HE3 | 1:75:A:LYS:HG3 | 7 | 0.14 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 4 | 0.14 |
| (3,450) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 5 | 0.14 |
| (3,423) | 1:61:A:LEU:HD11 | 1:25:A:THR:H | 7 | 0.14 |
| (3,353) | 1:28:A:LEU:HD21 | 1:28:A:LEU:HB3 | 6 | 0.14 |
| (3,332) | 1:43:A:ILE:HG21 | 1:43:A:ILE:HG13 | 1 | 0.14 |
| (3,312) | 1:106:A:GLU:HG2 | 1:106:A:GLU:H | 3 | 0.14 |
| (3,310) | 1:111:A:LYS:HD2 | 1:111:A:LYS:HG2 | 4 | 0.14 |
| (3,310) | 1:111:A:LYS:HD2 | 1:111:A:LYS:HG2 | 9 | 0.14 |
| (3,272) | 1:47:A:THR:HG23 | 1:62:A:ASP:HA | 3 | 0.14 |
| (3,180) | 1:65:A:HIS:H | 1:62:A:ASP:HB3 | 7 | 0.14 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 10 | 0.14 |
| (3,69) | 1:66:A:LEU:HD13 | 1:21:A:VAL:HB | 1 | 0.14 |
| (3,69) | 1:66:A:LEU:HD11 | 1:21:A:VAL:HB | 3 | 0.14 |
| (3,60) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 1 | 0.14 |
| (3,60) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 4 | 0.14 |
| (3,60) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 6 | 0.14 |
| (3,60) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 9 | 0.14 |
| (3,60) | 1:53:A:ILE:HG21 | 1:53:A:ILE:HB | 10 | 0.14 |
| (2,477) | 1:102:A:THR:H | 1:92:A:GLU:HG3 | 10 | 0.14 |
| (2,361) | 1:84:A:TYR:HB2 | 1:103:A:ILE:HG13 | 5 | 0.14 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG11 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG12 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG13 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG11 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG12 | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG13 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG11 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG12 | 9 | 0.14 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG13 | 9 | 0.14 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE1 | 1 | 0.14 |
| (1,3855) | 1:120:A:TYR:H | 1:120:A:TYR:HE2 | 1 | 0.14 |
| (1,3781) | 1:14:A:TRP:HA | 1:13:A:TYR:HD1 | 4 | 0.14 |
| (1,3781) | 1:14:A:TRP:HA | 1:13:A:TYR:HD2 | 4 | 0.14 |
| (1,3770) | 1:63:A:GLN:HE22 | 1:46:A:TYR:HD1 | 10 | 0.14 |
| (1,3770) | 1:63:A:GLN:HE22 | 1:46:A:TYR:HD2 | 10 | 0.14 |
| (1,3715) | 1:84:A:TYR:HE1 | 1:87:A:ASN:HD22 | 10 | 0.14 |
| (1,3715) | 1:84:A:TYR:HE2 | 1:87:A:ASN:HD22 | 10 | 0.14 |
| (1,3676) | 1:49:A:VAL:H | 1:43:A:ILE:HB | 1 | 0.14 |
| (1,3670) | 1:48:A:ALA:H | 1:42:A:VAL:HA | 10 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB1 | 1:42:A:VAL:H | 6 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB2 | 1:42:A:VAL:H | 6 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB3 | 1:42:A:VAL:H | 6 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB1 | 1:42:A:VAL:H | 7 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB2 | 1:42:A:VAL:H | 7 | 0.14 |
| (1,3665) | 1:48:A:ALA:HB3 | 1:42:A:VAL:H | 7 | 0.14 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 4 | 0.14 |
| (1,3600) | 1:110:A:LEU:H | 1:111:A:LYS:HA | 2 | 0.14 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 1 | 0.14 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 1 | 0.14 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 1 | 0.14 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 1 | 0.14 |
| (1,3511) | 1:43:A:ILE:H | 1:41:A:GLU:HG3 | 10 | 0.14 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD11 | 9 | 0.14 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD12 | 9 | 0.14 |
| (1,3309) | 1:23:A:ILE:H | 1:23:A:ILE:HD13 | 9 | 0.14 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 1 | 0.14 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 5 | 0.14 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 10 | 0.14 |
| (1,3245) | 1:30:A:GLU:HG2 | 1:33:A:HIS:H | 6 | 0.14 |
| (1,3163) | 1:49:A:VAL:HG21 | 1:41:A:GLU:H | 6 | 0.14 |
| (1,3163) | 1:49:A:VAL:HG22 | 1:41:A:GLU:H | 6 | 0.14 |
| (1,3163) | 1:49:A:VAL:HG23 | 1:41:A:GLU:H | 6 | 0.14 |
| (1,3100) | 1:48:A:ALA:HB1 | 1:47:A:THR:H | 7 | 0.14 |
| (1,3100) | 1:48:A:ALA:HB2 | 1:47:A:THR:H | 7 | 0.14 |
| (1,3100) | 1:48:A:ALA:HB3 | 1:47:A:THR:H | 7 | 0.14 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 6 | 0.14 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2750) | 1:79:A:VAL:HG21 | 1:86:A:GLY:H | 5 | 0.14 |
| (1,2750) | 1:79:A:VAL:HG22 | 1:86:A:GLY:H | 5 | 0.14 |
| (1,2750) | 1:79:A:VAL:HG23 | 1:86:A:GLY:H | 5 | 0.14 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 4 | 0.14 |
| (1,2732) | 1:84:A:TYR:HB2 | 1:87:A:ASN:H | 10 | 0.14 |
| (1,2675) | 1:92:A:GLU:H | 1:91:A:LEU:HG | 8 | 0.14 |
| (1,2641) | 1:95:A:ASN:HD21 | 1:95:A:ASN:H | 4 | 0.14 |
| (1,2640) | 1:102:A:THR:H | 1:95:A:ASN:H | 2 | 0.14 |
| (1,2625) | 1:97:A:LYS:H | 1:99:A:PHE:H | 8 | 0.14 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 7 | 0.14 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 1 | 0.14 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 8 | 0.14 |
| (1,2465) | 1:113:A:ARG:HB3 | 1:113:A:ARG:H | 10 | 0.14 |
| (1,2461) | 1:84:A:TYR:HE1 | 1:113:A:ARG:H | 1 | 0.14 |
| (1,2461) | 1:84:A:TYR:HE2 | 1:113:A:ARG:H | 1 | 0.14 |
| (1,2459) | 1:113:A:ARG:H | 1:107:A:THR:H | 10 | 0.14 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 6 | 0.14 |
| (1,2441) | 1:84:A:TYR:HE1 | 1:116:A:GLU:H | 8 | 0.14 |
| (1,2441) | 1:84:A:TYR:HE2 | 1:116:A:GLU:H | 8 | 0.14 |
| (1,2411) | 1:118:A:ILE:H | 1:101:A:ALA:HA | 4 | 0.14 |
| (1,2400) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 7 | 0.14 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 2 | 0.14 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 4 | 0.14 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 7 | 0.14 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG11 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG12 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG13 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG11 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG12 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG13 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG11 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG12 | 6 | 0.14 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG13 | 6 | 0.14 |
| (1,2221) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HA | 8 | 0.14 |
| (1,2221) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HA | 8 | 0.14 |
| (1,2221) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HA | 8 | 0.14 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB1 | 2 | 0.14 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB2 | 2 | 0.14 |
| (1,2219) | 1:120:A:TYR:H | 1:101:A:ALA:HB3 | 2 | 0.14 |
| (1,2218) | 1:102:A:THR:HB | 1:103:A:ILE:H | 1 | 0.14 |
| (1,2218) | 1:102:A:THR:HB | 1:103:A:ILE:H | 7 | 0.14 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 4 | 0.14 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 4 | 0.14 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 9 | 0.14 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 9 | 0.14 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 9 | 0.14 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 9 | 0.14 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 9 | 0.14 |
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 9 | 0.14 |
| (1,2197) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 9 | 0.14 |
| (1,2194) | 1:107:A:THR:HG21 | 1:87:A:ASN:HA | 10 | 0.14 |
| (1,2194) | 1:107:A:THR:HG22 | 1:87:A:ASN:HA | 10 | 0.14 |
| (1,2194) | 1:107:A:THR:HG23 | 1:87:A:ASN:HA | 10 | 0.14 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 9 | 0.14 |
| (1,2128) | 1:70:A:ILE:HD11 | 1:121:A:GLU:HA | 9 | 0.14 |
| (1,2128) | 1:70:A:ILE:HD12 | 1:121:A:GLU:HA | 9 | 0.14 |
| (1,2128) | 1:70:A:ILE:HD13 | 1:121:A:GLU:HA | 9 | 0.14 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 2 | 0.14 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 2 | 0.14 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 2 | 0.14 |
| (1,2049) | 1:19:A:ILE:HB | 1:124:A:SER:HB2 | 4 | 0.14 |
| (1,2049) | 1:19:A:ILE:HB | 1:124:A:SER:HB2 | 5 | 0.14 |
| (1,2049) | 1:19:A:ILE:HB | 1:124:A:SER:HB2 | 8 | 0.14 |
| (1,1950) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 2 | 0.14 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 2 | 0.14 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 7 | 0.14 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 7 | 0.14 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 7 | 0.14 |
| (1,1882) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 10 | 0.14 |
| (1,1765) | 1:105:A:ILE:HG21 | 1:87:A:ASN:HB2 | 6 | 0.14 |
| (1,1765) | 1:105:A:ILE:HG22 | 1:87:A:ASN:HB2 | 6 | 0.14 |
| (1,1765) | 1:105:A:ILE:HG23 | 1:87:A:ASN:HB2 | 6 | 0.14 |
| (1,1688) | 1:103:A:ILE:HB | 1:103:A:ILE:H | 10 | 0.14 |
| (1,1678) | 1:102:A:THR:HG21 | 1:103:A:ILE:HA | 4 | 0.14 |
| (1,1678) | 1:102:A:THR:HG22 | 1:103:A:ILE:HA | 4 | 0.14 |
| (1,1678) | 1:102:A:THR:HG23 | 1:103:A:ILE:HA | 4 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB1 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB2 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD21 | 1:101:A:ALA:HB3 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB1 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB2 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD22 | 1:101:A:ALA:HB3 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB1 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB2 | 7 | 0.14 |
| (1,1663) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 7 | 0.14 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 7 | 0.14 |
| (1,1616) | 1:98:A:THR:HG21 | 1:98:A:THR:H | 7 | 0.14 |
| (1,1616) | 1:98:A:THR:HG22 | 1:98:A:THR:H | 7 | 0.14 |
| (1,1616) | 1:98:A:THR:HG23 | 1:98:A:THR:H | 7 | 0.14 |
| (1,1611) | 1:98:A:THR:HA | 1:98:A:THR:HB | 5 | 0.14 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 9 | 0.14 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 9 | 0.14 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 9 | 0.14 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 2 | 0.14 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD11 | 2 | 0.14 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD12 | 2 | 0.14 |
| (1,1518) | 1:75:A:LYS:H | 1:91:A:LEU:HD13 | 2 | 0.14 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 5 | 0.14 |
| (1,1434) | 1:85:A:ARG:HA | 1:81:A:ASN:HA | 5 | 0.14 |
| (1,1386) | 1:81:A:ASN:HA | 1:81:A:ASN:HB2 | 4 | 0.14 |
| (1,1352) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA2 | 8 | 0.14 |
| (1,1352) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA2 | 8 | 0.14 |
| (1,1352) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA2 | 8 | 0.14 |
| (1,1306) | 1:77:A:ILE:HD11 | 1:90:A:THR:HA | 5 | 0.14 |
| (1,1306) | 1:77:A:ILE:HD12 | 1:90:A:THR:HA | 5 | 0.14 |
| (1,1306) | 1:77:A:ILE:HD13 | 1:90:A:THR:HA | 5 | 0.14 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 2 | 0.14 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 2 | 0.14 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 2 | 0.14 |
| (1,1223) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 2 | 0.14 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 4 | 0.14 |
| (1,971) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 5 | 0.14 |
| (1,922) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 6 | 0.14 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG21 | 3 | 0.14 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG22 | 3 | 0.14 |
| (1,889) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HG23 | 3 | 0.14 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD11 | 4 | 0.14 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD12 | 4 | 0.14 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD13 | 4 | 0.14 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 5 | 0.14 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 2 | 0.14 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 7 | 0.14 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG11 | 2 | 0.14 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG12 | 2 | 0.14 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG13 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,530) | 1:37:A:ALA:HB1 | 1:38:A:ILE:H | 3 | 0.14 |
| (1,530) | 1:37:A:ALA:HB2 | 1:38:A:ILE:H | 3 | 0.14 |
| (1,530) | 1:37:A:ALA:HB3 | 1:38:A:ILE:H | 3 | 0.14 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 10 | 0.14 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 2 | 0.14 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 2 | 0.14 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 2 | 0.14 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 2 | 0.14 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 2 | 0.14 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 2 | 0.14 |
| (1,439) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 1 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 3 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD21 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD22 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD11 | 1:91:A:LEU:HD23 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD21 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD22 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD12 | 1:91:A:LEU:HD23 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD21 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD22 | 9 | 0.14 |
| (1,430) | 1:91:A:LEU:HD13 | 1:91:A:LEU:HD23 | 9 | 0.14 |
| (1,375) | 1:23:A:ILE:HG21 | 1:66:A:LEU:HA | 3 | 0.14 |
| (1,375) | 1:23:A:ILE:HG22 | 1:66:A:LEU:HA | 3 | 0.14 |
| (1,375) | 1:23:A:ILE:HG23 | 1:66:A:LEU:HA | 3 | 0.14 |
| (1,288) | 1:20:A:ILE:H | 1:20:A:ILE:HG12 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 6 | 0.14 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 6 | 0.14 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 6 | 0.14 |
| (1,154) | 1:16:A:GLN:HA | 1:16:A:GLN:HB3 | 3 | 0.14 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 3 | 0.14 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 3 | 0.14 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 3 | 0.14 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 5 | 0.14 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 5 | 0.14 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 5 | 0.14 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD11 | 7 | 0.14 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD12 | 7 | 0.14 |
| (1,106) | 1:14:A:TRP:HB3 | 1:80:A:LEU:HD13 | 7 | 0.14 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 3 | 0.14 |
| (1,24) | 1:7:A:ARG:HA | 1:7:A:ARG:HB3 | 8 | 0.14 |
| (1,24) | 1:7:A:ARG:HA | 1:7:A:ARG:HB3 | 9 | 0.14 |
| (3,1182) | 1:98:A:THR:HG23 | 1:98:A:THR:HA | 7 | 0.13 |
| (3,1167) | 1:115:A:VAL:HG22 | 1:115:A:VAL:HB | 3 | 0.13 |
| (3,1167) | 1:115:A:VAL:HG22 | 1:115:A:VAL:HB | 5 | 0.13 |
| (3,1167) | 1:115:A:VAL:HG21 | 1:115:A:VAL:HB | 6 | 0.13 |
| (3,1167) | 1:115:A:VAL:HG22 | 1:115:A:VAL:HB | 10 | 0.13 |
| (3,1135) | 1:79:A:VAL:H | 1:123:A:ILE:HG22 | 7 | 0.13 |
| (3,1053) | 1:21:A:VAL:HG23 | 1:66:A:LEU:HD21 | 8 | 0.13 |
| (3,965) | 1:95:A:ASN:H | 1:101:A:ALA:H | 1 | 0.13 |
| (3,890) | 1:68:A:THR:HB | 1:124:A:SER:H | 9 | 0.13 |
| (3,855) | 1:17:A:PRO:HD2 | 1:16:A:GLN:HB2 | 2 | 0.13 |
| (3,855) | 1:17:A:PRO:HD3 | 1:16:A:GLN:HB2 | 8 | 0.13 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 1 | 0.13 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 5 | 0.13 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 8 | 0.13 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 9 | 0.13 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 10 | 0.13 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 8 | 0.13 |
| (3,823) | 1:123:A:ILE:HG13 | 1:123:A:ILE:HG21 | 9 | 0.13 |
| (3,817) | 1:84:A:TYR:HA | 1:85:A:ARG:H | 1 | 0.13 |
| (3,816) | 1:77:A:ILE:H | 1:91:A:LEU:H | 2 | 0.13 |
| (3,781) | 1:113:A:ARG:HD2 | 1:114:A:ARG:HA | 4 | 0.13 |
| (3,780) | 1:45:A:LYS:HA | 1:45:A:LYS:HD3 | 2 | 0.13 |
| (3,732) | 1:48:A:ALA:HB2 | 1:43:A:ILE:H | 1 | 0.13 |
| (3,729) | 1:26:A:LYS:HD2 | 1:26:A:LYS:HE3 | 4 | 0.13 |
| (3,729) | 1:26:A:LYS:HD2 | 1:26:A:LYS:HE3 | 8 | 0.13 |
| (3,729) | 1:26:A:LYS:HD2 | 1:26:A:LYS:HE3 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,655) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HD3 | 1 | 0.13 |
| (3,655) | 1:26:A:LYS:HG3 | 1:26:A:LYS:HD2 | 10 | 0.13 |
| (3,580) | 1:92:A:GLU:HB3 | 1:92:A:GLU:HA | 2 | 0.13 |
| (3,580) | 1:92:A:GLU:HB3 | 1:92:A:GLU:HA | 8 | 0.13 |
| (3,567) | 1:89:A:GLY:HA2 | 1:105:A:ILE:HD13 | 9 | 0.13 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 1 | 0.13 |
| (3,310) | 1:111:A:LYS:HD3 | 1:111:A:LYS:HG3 | 5 | 0.13 |
| (3,310) | 1:51:A:LYS:HD2 | 1:51:A:LYS:HG3 | 10 | 0.13 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD13 | 10 | 0.13 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 1 | 0.13 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 7 | 0.13 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 7 | 0.13 |
| (3,69) | 1:66:A:LEU:HD12 | 1:21:A:VAL:HB | 9 | 0.13 |
| (3,60) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 3 | 0.13 |
| (3,60) | 1:53:A:ILE:HG22 | 1:53:A:ILE:HB | 5 | 0.13 |
| (3,60) | 1:53:A:ILE:HG23 | 1:53:A:ILE:HB | 7 | 0.13 |
| (2,626) | 1:48:A:ALA:H | 1:60:A:LYS:HE3 | 2 | 0.13 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 8 | 0.13 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 8 | 0.13 |
| (1,3684) | 1:50:A:VAL:HG21 | 1:60:A:LYS:H | 10 | 0.13 |
| (1,3684) | 1:50:A:VAL:HG22 | 1:60:A:LYS:H | 10 | 0.13 |
| (1,3684) | 1:50:A:VAL:HG23 | 1:60:A:LYS:H | 10 | 0.13 |
| (1,3665) | 1:48:A:ALA:HB1 | 1:42:A:VAL:H | 5 | 0.13 |
| (1,3665) | 1:48:A:ALA:HB2 | 1:42:A:VAL:H | 5 | 0.13 |
| (1,3665) | 1:48:A:ALA:HB3 | 1:42:A:VAL:H | 5 | 0.13 |
| (1,3642) | 1:13:A:TYR:H | 1:45:A:LYS:HB2 | 4 | 0.13 |
| (1,3631) | 1:23:A:ILE:H | 1:32:A:TYR:HB3 | 5 | 0.13 |
| (1,3631) | 1:23:A:ILE:H | 1:32:A:TYR:HB3 | 6 | 0.13 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 1 | 0.13 |
| (1,3612) | 1:119:A:GLN:HB3 | 1:119:A:GLN:HE21 | 5 | 0.13 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 8 | 0.13 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 8 | 0.13 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 8 | 0.13 |
| (1,3537) | 1:46:A:TYR:HE1 | 1:63:A:GLN:HE21 | 5 | 0.13 |
| (1,3537) | 1:46:A:TYR:HE2 | 1:63:A:GLN:HE21 | 5 | 0.13 |
| (1,3537) | 1:46:A:TYR:HE1 | 1:63:A:GLN:HE21 | 8 | 0.13 |
| (1,3537) | 1:46:A:TYR:HE2 | 1:63:A:GLN:HE21 | 8 | 0.13 |
| (1,3520) | 1:52:A:MET:HG2 | 1:59:A:LEU:H | 2 | 0.13 |
| (1,3501) | 1:40:A:LYS:HE3 | 1:38:A:ILE:H | 4 | 0.13 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 8 | 0.13 |
| (1,3453) | 1:14:A:TRP:HA | 1:16:A:GLN:HE22 | 3 | 0.13 |
| (1,3446) | 1:68:A:THR:HG21 | 1:14:A:TRP:HE1 | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3446) | 1:68:A:THR:HG22 | 1:14:A:TRP:HE1 | 6 | 0.13 |
| (1,3446) | 1:68:A:THR:HG23 | 1:14:A:TRP:HE1 | 6 | 0.13 |
| (1,3402) | 1:9:A:ALA:HA | 1:10:A:ARG:H | 6 | 0.13 |
| (1,3389) | 1:82:A:GLY:H | 1:11:A:THR:H | 9 | 0.13 |
| (1,3265) | 1:29:A:GLY:H | 1:28:A:LEU:HB2 | 6 | 0.13 |
| (1,3255) | 1:31:A:LYS:HG3 | 1:32:A:TYR:H | 5 | 0.13 |
| (1,3225) | 1:35:A:LYS:H | 1:34:A:LYS:HG3 | 7 | 0.13 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD11 | 6 | 0.13 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD12 | 6 | 0.13 |
| (1,3209) | 1:36:A:LYS:H | 1:53:A:ILE:HD13 | 6 | 0.13 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG21 | 3 | 0.13 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG22 | 3 | 0.13 |
| (1,3136) | 1:44:A:ASP:H | 1:42:A:VAL:HG23 | 3 | 0.13 |
| (1,2876) | 1:73:A:PRO:HD2 | 1:72:A:ALA:H | 10 | 0.13 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 3 | 0.13 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 7 | 0.13 |
| (1,2775) | 1:82:A:GLY:H | 1:83:A:GLY:H | 9 | 0.13 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD11 | 8 | 0.13 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD12 | 8 | 0.13 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD13 | 8 | 0.13 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 4 | 0.13 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 4 | 0.13 |
| (1,2461) | 1:84:A:TYR:HE1 | 1:113:A:ARG:H | 6 | 0.13 |
| (1,2461) | 1:84:A:TYR:HE2 | 1:113:A:ARG:H | 6 | 0.13 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 3 | 0.13 |
| (1,2448) | 1:115:A:VAL:H | 1:103:A:ILE:HG13 | 2 | 0.13 |
| (1,2368) | 1:119:A:GLN:HA | 1:121:A:GLU:H | 4 | 0.13 |
| (1,2368) | 1:119:A:GLN:HA | 1:121:A:GLU:H | 7 | 0.13 |
| (1,2335) | 1:68:A:THR:HB | 1:125:A:LYS:H | 7 | 0.13 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 3 | 0.13 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 10 | 0.13 |
| (1,2298) | 1:14:A:TRP:H | 1:13:A:TYR:HB3 | 4 | 0.13 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 1 | 0.13 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 1 | 0.13 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 1 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG21 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG22 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG11 | 1:123:A:ILE:HG23 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG21 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG22 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG12 | 1:123:A:ILE:HG23 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG21 | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG22 | 5 | 0.13 |
| (1,2240) | 1:79:A:VAL:HG13 | 1:123:A:ILE:HG23 | 5 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 1 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 1 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 1 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 2 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 2 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 2 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 5 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 5 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 5 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 6 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 6 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 6 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 10 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 10 | 0.13 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 10 | 0.13 |
| (1,2197) | 1:106:A:GLU:HB2 | 1:105:A:ILE:HA | 8 | 0.13 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 3 | 0.13 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 3 | 0.13 |
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 3 | 0.13 |
| (1,1966) | 1:118:A:ILE:HG21 | 1:122:A:ASP:H | 7 | 0.13 |
| (1,1966) | 1:118:A:ILE:HG22 | 1:122:A:ASP:H | 7 | 0.13 |
| (1,1966) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 7 | 0.13 |
| (1,1965) | 1:118:A:ILE:HG12 | 1:118:A:ILE:H | 6 | 0.13 |
| (1,1960) | 1:118:A:ILE:HG13 | 1:118:A:ILE:H | 1 | 0.13 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG11 | 10 | 0.13 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG12 | 10 | 0.13 |
| (1,1924) | 1:113:A:ARG:HB3 | 1:115:A:VAL:HG13 | 10 | 0.13 |
| (1,1870) | 1:113:A:ARG:HA | 1:113:A:ARG:HD2 | 4 | 0.13 |
| (1,1785) | 1:107:A:THR:HB | 1:107:A:THR:HA | 1 | 0.13 |
| (1,1777) | 1:106:A:GLU:HB3 | 1:106:A:GLU:H | 9 | 0.13 |
| (1,1716) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 5 | 0.13 |
| (1,1716) | 1:103:A:ILE:HG22 | 1:102:A:THR:HA | 5 | 0.13 |
| (1,1716) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 5 | 0.13 |
| (1,1702) | 1:84:A:TYR:HB2 | 1:103:A:ILE:HD11 | 5 | 0.13 |
| (1,1702) | 1:84:A:TYR:HB2 | 1:103:A:ILE:HD12 | 5 | 0.13 |
| (1,1702) | 1:84:A:TYR:HB2 | 1:103:A:ILE:HD13 | 5 | 0.13 |
| (1,1638) | 1:118:A:ILE:H | 1:100:A:SER:HB2 | 7 | 0.13 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 9 | 0.13 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 10 | 0.13 |
| (1,1611) | 1:98:A:THR:HA | 1:98:A:THR:HB | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1607) | 1:97:A:LYS:HB3 | 1:97:A:LYS:HA | 1 | 0.13 |
| (1,1585) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 10 | 0.13 |
| (1,1585) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 10 | 0.13 |
| (1,1585) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 10 | 0.13 |
| (1,1552) | 1:93:A:SER:HA | 1:94:A:ILE:H | 10 | 0.13 |
| (1,1537) | 1:97:A:LYS:HB3 | 1:98:A:THR:H | 9 | 0.13 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD11 | 3 | 0.13 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD12 | 3 | 0.13 |
| (1,1519) | 1:73:A:PRO:HA | 1:91:A:LEU:HD13 | 3 | 0.13 |
| (1,1386) | 1:81:A:ASN:HA | 1:81:A:ASN:HB2 | 3 | 0.13 |
| (1,1352) | 1:90:A:THR:HG21 | 1:74:A:GLY:HA2 | 9 | 0.13 |
| (1,1352) | 1:90:A:THR:HG22 | 1:74:A:GLY:HA2 | 9 | 0.13 |
| (1,1352) | 1:90:A:THR:HG23 | 1:74:A:GLY:HA2 | 9 | 0.13 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 3 | 0.13 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 3 | 0.13 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 3 | 0.13 |
| (1,1351) | 1:48:A:ALA:HB1 | 1:42:A:VAL:HA | 4 | 0.13 |
| (1,1351) | 1:48:A:ALA:HB2 | 1:42:A:VAL:HA | 4 | 0.13 |
| (1,1351) | 1:48:A:ALA:HB3 | 1:42:A:VAL:HA | 4 | 0.13 |
| (1,1315) | 1:31:A:LYS:HG2 | 1:31:A:LYS:H | 5 | 0.13 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 3 | 0.13 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 3 | 0.13 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 3 | 0.13 |
| (1,1301) | 1:125:A:LYS:HA | 1:77:A:ILE:HB | 3 | 0.13 |
| (1,1223) | 1:73:A:PRO:HA | 1:91:A:LEU:HG | 3 | 0.13 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 2 | 0.13 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 5 | 0.13 |
| (1,1209) | 1:73:A:PRO:HD2 | 1:72:A:ALA:HA | 10 | 0.13 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG21 | 8 | 0.13 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG22 | 8 | 0.13 |
| (1,1200) | 1:71:A:PRO:HD3 | 1:70:A:ILE:HG23 | 8 | 0.13 |
| (1,1108) | 1:24:A:ILE:HD11 | 1:67:A:GLU:HB3 | 10 | 0.13 |
| (1,1108) | 1:24:A:ILE:HD12 | 1:67:A:GLU:HB3 | 10 | 0.13 |
| (1,1108) | 1:24:A:ILE:HD13 | 1:67:A:GLU:HB3 | 10 | 0.13 |
| (1,1021) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 2 | 0.13 |
| (1,1021) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 2 | 0.13 |
| (1,1021) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 2 | 0.13 |
| (1,970) | 1:61:A:LEU:HB2 | 1:62:A:ASP:H | 3 | 0.13 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 1 | 0.13 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 1 | 0.13 |
| (1,888) | 1:54:A:ASP:HB2 | 1:53:A:ILE:HB | 6 | 0.13 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 4 | 0.13 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 6 | 0.13 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 9 | 0.13 |
| (1,788) | 1:49:A:VAL:HG21 | 1:48:A:ALA:HA | 5 | 0.13 |
| (1,788) | 1:49:A:VAL:HG22 | 1:48:A:ALA:HA | 5 | 0.13 |
| (1,788) | 1:49:A:VAL:HG23 | 1:48:A:ALA:HA | 5 | 0.13 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 5 | 0.13 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 5 | 0.13 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 5 | 0.13 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 5 | 0.13 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 5 | 0.13 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 5 | 0.13 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 6 | 0.13 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 6 | 0.13 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 6 | 0.13 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 5 | 0.13 |
| (1,602) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HG21 | 10 | 0.13 |
| (1,602) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HG22 | 10 | 0.13 |
| (1,602) | 1:40:A:LYS:HE3 | 1:38:A:ILE:HG23 | 10 | 0.13 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 9 | 0.13 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 9 | 0.13 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 9 | 0.13 |
| (1,574) | 1:39:A:VAL:HG11 | 1:40:A:LYS:H | 4 | 0.13 |
| (1,574) | 1:39:A:VAL:HG12 | 1:40:A:LYS:H | 4 | 0.13 |
| (1,574) | 1:39:A:VAL:HG13 | 1:40:A:LYS:H | 4 | 0.13 |
| (1,530) | 1:37:A:ALA:HB1 | 1:38:A:ILE:H | 9 | 0.13 |
| (1,530) | 1:37:A:ALA:HB2 | 1:38:A:ILE:H | 9 | 0.13 |
| (1,530) | 1:37:A:ALA:HB3 | 1:38:A:ILE:H | 9 | 0.13 |
| (1,530) | 1:37:A:ALA:HB1 | 1:38:A:ILE:H | 10 | 0.13 |
| (1,530) | 1:37:A:ALA:HB2 | 1:38:A:ILE:H | 10 | 0.13 |
| (1,530) | 1:37:A:ALA:HB3 | 1:38:A:ILE:H | 10 | 0.13 |
| (1,479) | 1:31:A:LYS:HA | 1:32:A:TYR:H | 2 | 0.13 |
| (1,479) | 1:31:A:LYS:HA | 1:32:A:TYR:H | 10 | 0.13 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 10 | 0.13 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD11 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD12 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD21 | 1:59:A:LEU:HD13 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD11 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD12 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD22 | 1:59:A:LEU:HD13 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD11 | 3 | 0.13 |
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD12 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,456) | 1:61:A:LEU:HD23 | 1:59:A:LEU:HD13 | 3 | 0.13 |
| (1,455) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HB3 | 9 | 0.13 |
| (1,455) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HB3 | 9 | 0.13 |
| (1,455) | 1:28:A:LEU:HD13 | 1:28:A:LEU:HB3 | 9 | 0.13 |
| (1,439) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 7 | 0.13 |
| (1,439) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 8 | 0.13 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 4 | 0.13 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 4 | 0.13 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 4 | 0.13 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 3 | 0.13 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 3 | 0.13 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 3 | 0.13 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 6 | 0.13 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 6 | 0.13 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 6 | 0.13 |
| (1,354) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HD1 | 10 | 0.13 |
| (1,354) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HD2 | 10 | 0.13 |
| (1,354) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HD1 | 10 | 0.13 |
| (1,354) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HD2 | 10 | 0.13 |
| (1,354) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HD1 | 10 | 0.13 |
| (1,354) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HD2 | 10 | 0.13 |
| (1,281) | 1:20:A:ILE:HD11 | 1:20:A:ILE:HB | 7 | 0.13 |
| (1,281) | 1:20:A:ILE:HD12 | 1:20:A:ILE:HB | 7 | 0.13 |
| (1,281) | 1:20:A:ILE:HD13 | 1:20:A:ILE:HB | 7 | 0.13 |
| (1,281) | 1:20:A:ILE:HD11 | 1:20:A:ILE:HB | 9 | 0.13 |
| (1,281) | 1:20:A:ILE:HD12 | 1:20:A:ILE:HB | 9 | 0.13 |
| (1,281) | 1:20:A:ILE:HD13 | 1:20:A:ILE:HB | 9 | 0.13 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 5 | 0.13 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 5 | 0.13 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 5 | 0.13 |
| (1,248) | 1:19:A:ILE:HD11 | 1:14:A:TRP:HZ3 | 2 | 0.13 |
| (1,248) | 1:19:A:ILE:HD12 | 1:14:A:TRP:HZ3 | 2 | 0.13 |
| (1,248) | 1:19:A:ILE:HD13 | 1:14:A:TRP:HZ3 | 2 | 0.13 |
| (1,248) | 1:19:A:ILE:HD11 | 1:14:A:TRP:HZ3 | 3 | 0.13 |
| (1,248) | 1:19:A:ILE:HD12 | 1:14:A:TRP:HZ3 | 3 | 0.13 |
| (1,248) | 1:19:A:ILE:HD13 | 1:14:A:TRP:HZ3 | 3 | 0.13 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 6 | 0.13 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 7 | 0.13 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 7 | 0.13 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 7 | 0.13 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 2 | 0.13 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 4 | 0.13 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 5 | 0.13 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 7 | 0.13 |
| (3,1184) | 1:55:A:SER:HB3 | 1:57:A:ASP:HB2 | 9 | 0.12 |
| (3,1167) | 1:115:A:VAL:HG23 | 1:115:A:VAL:HB | 1 | 0.12 |
| (3,1146) | 1:115:A:VAL:HA | 1:103:A:ILE:H | 7 | 0.12 |
| (3,1091) | 1:112:A:GLY:H | 1:105:A:ILE:H | 9 | 0.12 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG21 | 8 | 0.12 |
| (3,1033) | 1:79:A:VAL:H | 1:123:A:ILE:HG23 | 10 | 0.12 |
| (3,1017) | 1:23:A:ILE:H | 1:22:A:LYS:HG2 | 3 | 0.12 |
| (3,933) | 1:123:A:ILE:HD11 | 1:100:A:SER:HB2 | 10 | 0.12 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 2 | 0.12 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 3 | 0.12 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 4 | 0.12 |
| (3,844) | 1:106:A:GLU:H | 1:106:A:GLU:HA | 7 | 0.12 |
| (3,838) | 1:52:A:MET:H | 1:59:A:LEU:H | 9 | 0.12 |
| (3,820) | 1:93:A:SER:H | 1:92:A:GLU:HG2 | 8 | 0.12 |
| (3,817) | 1:84:A:TYR:HA | 1:85:A:ARG:H | 8 | 0.12 |
| (3,817) | 1:84:A:TYR:HA | 1:85:A:ARG:H | 10 | 0.12 |
| (3,775) | 1:126:A:LEU:H | 1:125:A:LYS:HE2 | 1 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 1 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 2 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 3 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 4 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 5 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 6 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 7 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 8 | 0.12 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 10 | 0.12 |
| (3,743) | 1:37:A:ALA:HB1 | 1:50:A:VAL:HA | 9 | 0.12 |
| (3,729) | 1:26:A:LYS:HE2 | 1:26:A:LYS:HD3 | 3 | 0.12 |
| (3,729) | 1:26:A:LYS:HD2 | 1:26:A:LYS:HE3 | 5 | 0.12 |
| (3,706) | 1:16:A:GLN:H | 1:15:A:LEU:HB3 | 4 | 0.12 |
| (3,583) | 1:125:A:LYS:HE2 | 1:20:A:ILE:HD12 | 3 | 0.12 |
| (3,516) | 1:118:A:ILE:HG13 | 1:117:A:GLY:HA2 | 9 | 0.12 |
| (3,485) | 1:127:A:ALA:H | 1:126:A:LEU:HB3 | 5 | 0.12 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 1 | 0.12 |
| (3,475) | 1:26:A:LYS:HE3 | 1:30:A:GLU:HA | 10 | 0.12 |
| (3,450) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 2 | 0.12 |
| (3,450) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 8 | 0.12 |
| (3,426) | 1:119:A:GLN:HA | 1:100:A:SER:H | 3 | 0.12 |
| (3,403) | 1:113:A:ARG:HB2 | 1:105:A:ILE:H | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,379) | 1:45:A:LYS:HA | 1:13:A:TYR:HD2 | 2 | 0.12 |
| (3,332) | 1:43:A:ILE:HG22 | 1:43:A:ILE:HG13 | 6 | 0.12 |
| (3,332) | 1:43:A:ILE:HG23 | 1:43:A:ILE:HG13 | 10 | 0.12 |
| (3,310) | 1:111:A:LYS:HD3 | 1:111:A:LYS:HG2 | 1 | 0.12 |
| (3,310) | 1:111:A:LYS:HD3 | 1:111:A:LYS:HG2 | 7 | 0.12 |
| (3,310) | 1:111:A:LYS:HD2 | 1:111:A:LYS:HG3 | 8 | 0.12 |
| (3,296) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB3 | 9 | 0.12 |
| (3,257) | 1:53:A:ILE:H | 1:53:A:ILE:HD13 | 7 | 0.12 |
| (3,224) | 1:103:A:ILE:HG22 | 1:101:A:ALA:H | 6 | 0.12 |
| (3,224) | 1:103:A:ILE:HG21 | 1:101:A:ALA:H | 10 | 0.12 |
| (3,211) | 1:118:A:ILE:H | 1:116:A:GLU:HB3 | 2 | 0.12 |
| (3,173) | 1:39:A:VAL:HG13 | 1:17:A:PRO:HG3 | 9 | 0.12 |
| (3,129) | 1:77:A:ILE:HD11 | 1:123:A:ILE:HB | 2 | 0.12 |
| (3,129) | 1:77:A:ILE:HD13 | 1:123:A:ILE:HB | 7 | 0.12 |
| (2,593) | 1:66:A:LEU:HB3 | 1:14:A:TRP:HE1 | 8 | 0.12 |
| (2,407) | 1:42:A:VAL:HG11 | 1:44:A:ASP:HA | 4 | 0.12 |
| (2,407) | 1:42:A:VAL:HG12 | 1:44:A:ASP:HA | 4 | 0.12 |
| (2,407) | 1:42:A:VAL:HG13 | 1:44:A:ASP:HA | 4 | 0.12 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG21 | 4 | 0.12 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG22 | 4 | 0.12 |
| (2,393) | 1:73:A:PRO:HG2 | 1:70:A:ILE:HG23 | 4 | 0.12 |
| (2,12) | 1:9:A:ALA:HA | 1:10:A:ARG:HD2 | 7 | 0.12 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD1 | 9 | 0.12 |
| (1,3775) | 1:13:A:TYR:HB2 | 1:46:A:TYR:HD2 | 9 | 0.12 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 4 | 0.12 |
| (1,3712) | 1:87:A:ASN:HD21 | 1:84:A:TYR:H | 5 | 0.12 |
| (1,3631) | 1:23:A:ILE:H | 1:32:A:TYR:HB3 | 9 | 0.12 |
| (1,3615) | 1:119:A:GLN:HE21 | 1:100:A:SER:HB2 | 9 | 0.12 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 9 | 0.12 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 9 | 0.12 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 9 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 2 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 3 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 5 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 6 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 7 | 0.12 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 10 | 0.12 |
| (1,3415) | 1:7:A:ARG:HG3 | 1:7:A:ARG:H | 9 | 0.12 |
| (1,3380) | 1:14:A:TRP:H | 1:13:A:TYR:HB3 | 4 | 0.12 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 2 | 0.12 |
| (1,3308) | 1:23:A:ILE:H | 1:23:A:ILE:HG12 | 6 | 0.12 |
| (1,3213) | 1:36:A:LYS:H | 1:35:A:LYS:H | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3213) | 1:36:A:LYS:H | 1:35:A:LYS:H | 3 | 0.12 |
| (1,3183) | 1:17:A:PRO:HA | 1:39:A:VAL:H | 7 | 0.12 |
| (1,3134) | 1:44:A:ASP:H | 1:43:A:ILE:HG13 | 7 | 0.12 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG21 | 1 | 0.12 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG22 | 1 | 0.12 |
| (1,3040) | 1:54:A:ASP:H | 1:53:A:ILE:HG23 | 1 | 0.12 |
| (1,3028) | 1:51:A:LYS:HG2 | 1:56:A:GLY:H | 2 | 0.12 |
| (1,3027) | 1:10:A:ARG:HB2 | 1:81:A:ASN:HD21 | 10 | 0.12 |
| (1,3000) | 1:59:A:LEU:HD11 | 1:60:A:LYS:H | 5 | 0.12 |
| (1,3000) | 1:59:A:LEU:HD12 | 1:60:A:LYS:H | 5 | 0.12 |
| (1,3000) | 1:59:A:LEU:HD13 | 1:60:A:LYS:H | 5 | 0.12 |
| (1,3000) | 1:59:A:LEU:HD11 | 1:60:A:LYS:H | 8 | 0.12 |
| (1,3000) | 1:59:A:LEU:HD12 | 1:60:A:LYS:H | 8 | 0.12 |
| (1,3000) | 1:59:A:LEU:HD13 | 1:60:A:LYS:H | 8 | 0.12 |
| (1,2967) | 1:46:A:TYR:HB2 | 1:63:A:GLN:H | 6 | 0.12 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 6 | 0.12 |
| (1,2880) | 1:75:A:LYS:HB3 | 1:72:A:ALA:H | 7 | 0.12 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 2 | 0.12 |
| (1,2816) | 1:85:A:ARG:HA | 1:79:A:VAL:H | 5 | 0.12 |
| (1,2802) | 1:81:A:ASN:HB3 | 1:80:A:LEU:H | 8 | 0.12 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD11 | 4 | 0.12 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD12 | 4 | 0.12 |
| (1,2769) | 1:84:A:TYR:H | 1:105:A:ILE:HD13 | 4 | 0.12 |
| (1,2750) | 1:79:A:VAL:HG21 | 1:86:A:GLY:H | 4 | 0.12 |
| (1,2750) | 1:79:A:VAL:HG22 | 1:86:A:GLY:H | 4 | 0.12 |
| (1,2750) | 1:79:A:VAL:HG23 | 1:86:A:GLY:H | 4 | 0.12 |
| (1,2736) | 1:79:A:VAL:HG21 | 1:87:A:ASN:H | 7 | 0.12 |
| (1,2736) | 1:79:A:VAL:HG22 | 1:87:A:ASN:H | 7 | 0.12 |
| (1,2736) | 1:79:A:VAL:HG23 | 1:87:A:ASN:H | 7 | 0.12 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 2 | 0.12 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 2 | 0.12 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 2 | 0.12 |
| (1,2658) | 1:91:A:LEU:HD11 | 1:94:A:ILE:H | 8 | 0.12 |
| (1,2658) | 1:91:A:LEU:HD12 | 1:94:A:ILE:H | 8 | 0.12 |
| (1,2658) | 1:91:A:LEU:HD13 | 1:94:A:ILE:H | 8 | 0.12 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 3 | 0.12 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 8 | 0.12 |
| (1,2633) | 1:96:A:GLU:H | 1:95:A:ASN:HB3 | 3 | 0.12 |
| (1,2607) | 1:97:A:LYS:HG2 | 1:98:A:THR:H | 3 | 0.12 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 7 | 0.12 |
| (1,2592) | 1:97:A:LYS:HB3 | 1:100:A:SER:H | 9 | 0.12 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2467) | 1:113:A:ARG:H | 1:105:A:ILE:HG13 | 5 | 0.12 |
| (1,2460) | 1:113:A:ARG:H | 1:111:A:LYS:H | 3 | 0.12 |
| (1,2448) | 1:115:A:VAL:H | 1:103:A:ILE:HG13 | 7 | 0.12 |
| (1,2437) | 1:118:A:ILE:HG13 | 1:116:A:GLU:H | 6 | 0.12 |
| (1,2397) | 1:122:A:ASP:HA | 1:119:A:GLN:H | 4 | 0.12 |
| (1,2328) | 1:126:A:LEU:H | 1:125:A:LYS:H | 1 | 0.12 |
| (1,2218) | 1:102:A:THR:HB | 1:103:A:ILE:H | 8 | 0.12 |
| (1,2218) | 1:102:A:THR:HB | 1:103:A:ILE:H | 10 | 0.12 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 3 | 0.12 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 3 | 0.12 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 3 | 0.12 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD11 | 7 | 0.12 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD12 | 7 | 0.12 |
| (1,2215) | 1:103:A:ILE:HA | 1:103:A:ILE:HD13 | 7 | 0.12 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD11 | 6 | 0.12 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD12 | 6 | 0.12 |
| (1,2211) | 1:84:A:TYR:HE1 | 1:103:A:ILE:HD13 | 6 | 0.12 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD11 | 6 | 0.12 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD12 | 6 | 0.12 |
| (1,2211) | 1:84:A:TYR:HE2 | 1:103:A:ILE:HD13 | 6 | 0.12 |
| (1,2207) | 1:103:A:ILE:HG21 | 1:118:A:ILE:HB | 3 | 0.12 |
| (1,2207) | 1:103:A:ILE:HG22 | 1:118:A:ILE:HB | 3 | 0.12 |
| (1,2207) | 1:103:A:ILE:HG23 | 1:118:A:ILE:HB | 3 | 0.12 |
| (1,2193) | 1:107:A:THR:HG21 | 1:87:A:ASN:HA | 6 | 0.12 |
| (1,2193) | 1:107:A:THR:HG22 | 1:87:A:ASN:HA | 6 | 0.12 |
| (1,2193) | 1:107:A:THR:HG23 | 1:87:A:ASN:HA | 6 | 0.12 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 5 | 0.12 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 6 | 0.12 |
| (1,1995) | 1:68:A:THR:HG21 | 1:121:A:GLU:HA | 9 | 0.12 |
| (1,1995) | 1:68:A:THR:HG22 | 1:121:A:GLU:HA | 9 | 0.12 |
| (1,1995) | 1:68:A:THR:HG23 | 1:121:A:GLU:HA | 9 | 0.12 |
| (1,1946) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HB3 | 1 | 0.12 |
| (1,1936) | 1:116:A:GLU:H | 1:116:A:GLU:HG2 | 1 | 0.12 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG21 | 9 | 0.12 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG22 | 9 | 0.12 |
| (1,1888) | 1:76:A:ARG:HD2 | 1:90:A:THR:HG23 | 9 | 0.12 |
| (1,1829) | 1:110:A:LEU:HA | 1:111:A:LYS:H | 2 | 0.12 |
| (1,1829) | 1:110:A:LEU:HA | 1:111:A:LYS:H | 9 | 0.12 |
| (1,1785) | 1:107:A:THR:HB | 1:107:A:THR:HA | 2 | 0.12 |
| (1,1777) | 1:106:A:GLU:HB3 | 1:106:A:GLU:H | 2 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 2 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG22 | 1:102:A:THR:HA | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1716) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 2 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG21 | 1:102:A:THR:HA | 8 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG22 | 1:102:A:THR:HA | 8 | 0.12 |
| (1,1716) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 8 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 9 | 0.12 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 9 | 0.12 |
| (1,1678) | 1:102:A:THR:HG21 | 1:103:A:ILE:HA | 7 | 0.12 |
| (1,1678) | 1:102:A:THR:HG22 | 1:103:A:ILE:HA | 7 | 0.12 |
| (1,1678) | 1:102:A:THR:HG23 | 1:103:A:ILE:HA | 7 | 0.12 |
| (1,1655) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 5 | 0.12 |
| (1,1655) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 5 | 0.12 |
| (1,1655) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 5 | 0.12 |
| (1,1647) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 6 | 0.12 |
| (1,1641) | 1:117:A:GLY:HA3 | 1:100:A:SER:HB2 | 6 | 0.12 |
| (1,1635) | 1:100:A:SER:HA | 1:100:A:SER:HB2 | 2 | 0.12 |
| (1,1616) | 1:98:A:THR:HG21 | 1:98:A:THR:H | 5 | 0.12 |
| (1,1616) | 1:98:A:THR:HG22 | 1:98:A:THR:H | 5 | 0.12 |
| (1,1616) | 1:98:A:THR:HG23 | 1:98:A:THR:H | 5 | 0.12 |
| (1,1611) | 1:98:A:THR:HA | 1:98:A:THR:HB | 10 | 0.12 |
| (1,1535) | 1:93:A:SER:HA | 1:91:A:LEU:HG | 3 | 0.12 |
| (1,1492) | 1:104:A:VAL:H | 1:90:A:THR:HB | 9 | 0.12 |
| (1,1441) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 4 | 0.12 |
| (1,1426) | 1:85:A:ARG:HA | 1:87:A:ASN:H | 7 | 0.12 |
| (1,1313) | 1:77:A:ILE:H | 1:77:A:ILE:HG12 | 10 | 0.12 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG11 | 7 | 0.12 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG12 | 7 | 0.12 |
| (1,1144) | 1:68:A:THR:HA | 1:69:A:VAL:HG13 | 7 | 0.12 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 5 | 0.12 |
| (1,1070) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 9 | 0.12 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG21 | 10 | 0.12 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG22 | 10 | 0.12 |
| (1,1051) | 1:63:A:GLN:HG2 | 1:64:A:THR:HG23 | 10 | 0.12 |
| (1,964) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 10 | 0.12 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 3 | 0.12 |
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,877) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 10 | 0.12 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 5 | 0.12 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 5 | 0.12 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 5 | 0.12 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 5 | 0.12 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 5 | 0.12 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 5 | 0.12 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD11 | 5 | 0.12 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD12 | 5 | 0.12 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD13 | 5 | 0.12 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 1 | 0.12 |
| (1,797) | 1:50:A:VAL:HB | 1:50:A:VAL:H | 5 | 0.12 |
| (1,788) | 1:49:A:VAL:HG21 | 1:48:A:ALA:HA | 10 | 0.12 |
| (1,788) | 1:49:A:VAL:HG22 | 1:48:A:ALA:HA | 10 | 0.12 |
| (1,788) | 1:49:A:VAL:HG23 | 1:48:A:ALA:HA | 10 | 0.12 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB1 | 3 | 0.12 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB2 | 3 | 0.12 |
| (1,780) | 1:15:A:LEU:HA | 1:48:A:ALA:HB3 | 3 | 0.12 |
| (1,747) | 1:46:A:TYR:HA | 1:46:A:TYR:HD1 | 10 | 0.12 |
| (1,747) | 1:46:A:TYR:HA | 1:46:A:TYR:HD2 | 10 | 0.12 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 10 | 0.12 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 10 | 0.12 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 10 | 0.12 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 1 | 0.12 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 2 | 0.12 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 7 | 0.12 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 2 | 0.12 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 2 | 0.12 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 2 | 0.12 |
| (1,558) | 1:48:A:ALA:HB1 | 1:39:A:VAL:HB | 10 | 0.12 |
| (1,558) | 1:48:A:ALA:HB2 | 1:39:A:VAL:HB | 10 | 0.12 |
| (1,558) | 1:48:A:ALA:HB3 | 1:39:A:VAL:HB | 10 | 0.12 |
| (1,530) | 1:37:A:ALA:HB1 | 1:38:A:ILE:H | 7 | 0.12 |
| (1,530) | 1:37:A:ALA:HB2 | 1:38:A:ILE:H | 7 | 0.12 |
| (1,530) | 1:37:A:ALA:HB3 | 1:38:A:ILE:H | 7 | 0.12 |
| (1,479) | 1:31:A:LYS:HA | 1:32:A:TYR:H | 1 | 0.12 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 1 | 0.12 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 8 | 0.12 |
| (1,439) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 6 | 0.12 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG21 | 5 | 0.12 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG22 | 5 | 0.12 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG23 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 2 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 2 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 2 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 3 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 3 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 3 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 8 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 8 | 0.12 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 8 | 0.12 |
| (1,286) | 1:20:A:ILE:HD11 | 1:127:A:ALA:H | 4 | 0.12 |
| (1,286) | 1:20:A:ILE:HD12 | 1:127:A:ALA:H | 4 | 0.12 |
| (1,286) | 1:20:A:ILE:HD13 | 1:127:A:ALA:H | 4 | 0.12 |
| (1,281) | 1:20:A:ILE:HD11 | 1:20:A:ILE:HB | 3 | 0.12 |
| (1,281) | 1:20:A:ILE:HD12 | 1:20:A:ILE:HB | 3 | 0.12 |
| (1,281) | 1:20:A:ILE:HD13 | 1:20:A:ILE:HB | 3 | 0.12 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG21 | 7 | 0.12 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG22 | 7 | 0.12 |
| (1,266) | 1:127:A:ALA:H | 1:19:A:ILE:HG23 | 7 | 0.12 |
| (1,265) | 1:19:A:ILE:HG21 | 1:18:A:GLU:H | 1 | 0.12 |
| (1,265) | 1:19:A:ILE:HG22 | 1:18:A:GLU:H | 1 | 0.12 |
| (1,265) | 1:19:A:ILE:HG23 | 1:18:A:GLU:H | 1 | 0.12 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 6 | 0.12 |
| (1,35) | 1:113:A:ARG:HG3 | 1:114:A:ARG:H | 10 | 0.12 |
| (3,1170) | 1:111:A:LYS:HB2 | 1:112:A:GLY:H | 9 | 0.11 |
| (3,1166) | 1:118:A:ILE:HG13 | 1:103:A:ILE:H | 1 | 0.11 |
| (3,1153) | 1:3:A:GLU:HA | 1:4:A:GLU:H | 9 | 0.11 |
| (3,1108) | 1:53:A:ILE:HB | 1:56:A:GLY:H | 8 | 0.11 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 2 | 0.11 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 6 | 0.11 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 7 | 0.11 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 10 | 0.11 |
| (3,1057) | 1:8:A:THR:HA | 1:8:A:THR:HG22 | 2 | 0.11 |
| (3,1053) | 1:21:A:VAL:HG23 | 1:66:A:LEU:HD22 | 7 | 0.11 |
| (3,915) | 1:76:A:ARG:H | 1:76:A:ARG:HB2 | 7 | 0.11 |
| (3,915) | 1:76:A:ARG:H | 1:76:A:ARG:HB2 | 9 | 0.11 |
| (3,899) | 1:35:A:LYS:HA | 1:35:A:LYS:H | 6 | 0.11 |
| (3,890) | 1:68:A:THR:HB | 1:124:A:SER:H | 6 | 0.11 |
| (3,867) | 1:17:A:PRO:HB3 | 1:18:A:GLU:H | 7 | 0.11 |
| (3,826) | 1:5:A:LYS:H | 1:5:A:LYS:HA | 3 | 0.11 |
| (3,816) | 1:77:A:ILE:H | 1:91:A:LEU:H | 10 | 0.11 |
| (3,792) | 1:126:A:LEU:HG | 1:126:A:LEU:HD21 | 8 | 0.11 |
| (3,756) | 1:103:A:ILE:HG13 | 1:103:A:ILE:HA | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,729) | 1:26:A:LYS:HE2 | 1:26:A:LYS:HD3 | 7 | 0.11 |
| (3,721) | 1:51:A:LYS:HG3 | 1:57:A:ASP:HA | 8 | 0.11 |
| (3,655) | 1:26:A:LYS:HG2 | 1:26:A:LYS:HD3 | 2 | 0.11 |
| (3,552) | 1:32:A:TYR:HE1 | 1:57:A:ASP:HB3 | 7 | 0.11 |
| (3,534) | 1:82:A:GLY:H | 1:81:A:ASN:H | 1 | 0.11 |
| (3,534) | 1:82:A:GLY:H | 1:81:A:ASN:H | 3 | 0.11 |
| (3,534) | 1:82:A:GLY:H | 1:81:A:ASN:H | 4 | 0.11 |
| (3,489) | 1:51:A:LYS:HE3 | 1:56:A:GLY:HA3 | 6 | 0.11 |
| (3,399) | 1:45:A:LYS:HG3 | 1:44:A:ASP:HA | 9 | 0.11 |
| (3,353) | 1:61:A:LEU:HD23 | 1:61:A:LEU:HB3 | 7 | 0.11 |
| (3,280) | 1:112:A:GLY:H | 1:111:A:LYS:HG3 | 1 | 0.11 |
| (3,167) | 1:118:A:ILE:HG23 | 1:122:A:ASP:H | 1 | 0.11 |
| (3,129) | 1:77:A:ILE:HD12 | 1:123:A:ILE:HB | 1 | 0.11 |
| (3,128) | 1:77:A:ILE:HD13 | 1:123:A:ILE:HG21 | 6 | 0.11 |
| (3,72) | 1:20:A:ILE:HG22 | 1:20:A:ILE:HG12 | 4 | 0.11 |
| (3,66) | 1:40:A:LYS:HA | 1:40:A:LYS:HB3 | 1 | 0.11 |
| (3,29) | 1:108:A:GLY:H | 1:108:A:GLY:HA3 | 2 | 0.11 |
| (3,29) | 1:108:A:GLY:H | 1:108:A:GLY:HA3 | 8 | 0.11 |
| (2,626) | 1:48:A:ALA:H | 1:60:A:LYS:HE3 | 6 | 0.11 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 4 | 0.11 |
| (2,531) | 1:69:A:VAL:H | 1:71:A:PRO:HD2 | 5 | 0.11 |
| (1,3867) | 1:100:A:SER:H | 1:120:A:TYR:HE1 | 9 | 0.11 |
| (1,3867) | 1:100:A:SER:H | 1:120:A:TYR:HE2 | 9 | 0.11 |
| (1,3752) | 1:34:A:LYS:HG2 | 1:33:A:HIS:HE1 | 8 | 0.11 |
| (1,3705) | 1:75:A:LYS:H | 1:91:A:LEU:HA | 7 | 0.11 |
| (1,3633) | 1:103:A:ILE:H | 1:116:A:GLU:HG2 | 2 | 0.11 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 5 | 0.11 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 5 | 0.11 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 5 | 0.11 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 7 | 0.11 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 7 | 0.11 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 7 | 0.11 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 1 | 0.11 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 4 | 0.11 |
| (1,3456) | 1:16:A:GLN:HG3 | 1:16:A:GLN:HE22 | 9 | 0.11 |
| (1,3445) | 1:64:A:THR:HG21 | 1:14:A:TRP:HE1 | 6 | 0.11 |
| (1,3445) | 1:64:A:THR:HG22 | 1:14:A:TRP:HE1 | 6 | 0.11 |
| (1,3445) | 1:64:A:THR:HG23 | 1:14:A:TRP:HE1 | 6 | 0.11 |
| (1,3443) | 1:63:A:GLN:HG3 | 1:14:A:TRP:HE1 | 10 | 0.11 |
| (1,3368) | 1:15:A:LEU:H | 1:13:A:TYR:HB3 | 6 | 0.11 |
| (1,3245) | 1:30:A:GLU:HG3 | 1:33:A:HIS:H | 8 | 0.11 |
| (1,3134) | 1:44:A:ASP:H | 1:43:A:ILE:HG13 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3100) | 1:48:A:ALA:HB1 | 1:47:A:THR:H | 5 | 0.11 |
| (1,3100) | 1:48:A:ALA:HB2 | 1:47:A:THR:H | 5 | 0.11 |
| (1,3100) | 1:48:A:ALA:HB3 | 1:47:A:THR:H | 5 | 0.11 |
| (1,3089) | 1:48:A:ALA:H | 1:63:A:GLN:HA | 1 | 0.11 |
| (1,3022) | 1:51:A:LYS:HG3 | 1:57:A:ASP:H | 1 | 0.11 |
| (1,2962) | 1:63:A:GLN:H | 1:62:A:ASP:H | 1 | 0.11 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 1 | 0.11 |
| (1,2930) | 1:66:A:LEU:H | 1:65:A:HIS:HB3 | 8 | 0.11 |
| (1,2865) | 1:75:A:LYS:H | 1:71:A:PRO:HB2 | 2 | 0.11 |
| (1,2788) | 1:81:A:ASN:H | 1:84:A:TYR:H | 3 | 0.11 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 10 | 0.11 |
| (1,2759) | 1:79:A:VAL:HG21 | 1:85:A:ARG:H | 9 | 0.11 |
| (1,2759) | 1:79:A:VAL:HG22 | 1:85:A:ARG:H | 9 | 0.11 |
| (1,2759) | 1:79:A:VAL:HG23 | 1:85:A:ARG:H | 9 | 0.11 |
| (1,2641) | 1:95:A:ASN:HD21 | 1:95:A:ASN:H | 5 | 0.11 |
| (1,2630) | 1:96:A:GLU:H | 1:98:A:THR:H | 6 | 0.11 |
| (1,2588) | 1:100:A:SER:H | 1:100:A:SER:HB3 | 9 | 0.11 |
| (1,2573) | 1:101:A:ALA:H | 1:100:A:SER:HB2 | 5 | 0.11 |
| (1,2571) | 1:117:A:GLY:HA2 | 1:101:A:ALA:H | 1 | 0.11 |
| (1,2529) | 1:105:A:ILE:HG13 | 1:105:A:ILE:H | 5 | 0.11 |
| (1,2509) | 1:107:A:THR:H | 1:88:A:GLU:H | 6 | 0.11 |
| (1,2507) | 1:107:A:THR:HB | 1:107:A:THR:H | 6 | 0.11 |
| (1,2400) | 1:119:A:GLN:H | 1:100:A:SER:HB2 | 5 | 0.11 |
| (1,2368) | 1:119:A:GLN:HA | 1:121:A:GLU:H | 3 | 0.11 |
| (1,2358) | 1:122:A:ASP:H | 1:121:A:GLU:HB2 | 2 | 0.11 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 9 | 0.11 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG11 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG12 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG21 | 1:21:A:VAL:HG13 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG11 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG12 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG22 | 1:21:A:VAL:HG13 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG11 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG12 | 5 | 0.11 |
| (1,2283) | 1:68:A:THR:HG23 | 1:21:A:VAL:HG13 | 5 | 0.11 |
| (1,2258) | 1:23:A:ILE:HD11 | 1:32:A:TYR:HA | 3 | 0.11 |
| (1,2258) | 1:23:A:ILE:HD12 | 1:32:A:TYR:HA | 3 | 0.11 |
| (1,2258) | 1:23:A:ILE:HD13 | 1:32:A:TYR:HA | 3 | 0.11 |
| (1,2241) | 1:71:A:PRO:HA | 1:70:A:ILE:HG21 | 10 | 0.11 |
| (1,2241) | 1:71:A:PRO:HA | 1:70:A:ILE:HG22 | 10 | 0.11 |
| (1,2241) | 1:71:A:PRO:HA | 1:70:A:ILE:HG23 | 10 | 0.11 |
| (1,2190) | 1:107:A:THR:HG21 | 1:106:A:GLU:H | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2190) | 1:107:A:THR:HG22 | 1:106:A:GLU:H | 4 | 0.11 |
| (1,2190) | 1:107:A:THR:HG23 | 1:106:A:GLU:H | 4 | 0.11 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 7 | 0.11 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 7 | 0.11 |
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 7 | 0.11 |
| (1,2155) | 1:118:A:ILE:HA | 1:101:A:ALA:H | 8 | 0.11 |
| (1,2149) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 1 | 0.11 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG21 | 7 | 0.11 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG22 | 7 | 0.11 |
| (1,2110) | 1:126:A:LEU:HB3 | 1:77:A:ILE:HG23 | 7 | 0.11 |
| (1,2102) | 1:126:A:LEU:HD21 | 1:77:A:ILE:H | 6 | 0.11 |
| (1,2102) | 1:126:A:LEU:HD22 | 1:77:A:ILE:H | 6 | 0.11 |
| (1,2102) | 1:126:A:LEU:HD23 | 1:77:A:ILE:H | 6 | 0.11 |
| (1,2049) | 1:19:A:ILE:HB | 1:124:A:SER:HB2 | 7 | 0.11 |
| (1,1947) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HA | 4 | 0.11 |
| (1,1896) | 1:114:A:ARG:HA | 1:114:A:ARG:HG2 | 9 | 0.11 |
| (1,1890) | 1:84:A:TYR:HE1 | 1:113:A:ARG:HD3 | 6 | 0.11 |
| (1,1890) | 1:84:A:TYR:HE2 | 1:113:A:ARG:HD3 | 6 | 0.11 |
| (1,1868) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 8 | 0.11 |
| (1,1868) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 8 | 0.11 |
| (1,1868) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 8 | 0.11 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD11 | 3 | 0.11 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD12 | 3 | 0.11 |
| (1,1836) | 1:110:A:LEU:HB2 | 1:105:A:ILE:HD13 | 3 | 0.11 |
| (1,1785) | 1:107:A:THR:HB | 1:107:A:THR:HA | 4 | 0.11 |
| (1,1753) | 1:115:A:VAL:HG11 | 1:105:A:ILE:HG13 | 2 | 0.11 |
| (1,1753) | 1:115:A:VAL:HG12 | 1:105:A:ILE:HG13 | 2 | 0.11 |
| (1,1753) | 1:115:A:VAL:HG13 | 1:105:A:ILE:HG13 | 2 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG21 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG22 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG21 | 1:123:A:ILE:HG23 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG21 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG22 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG22 | 1:123:A:ILE:HG23 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG21 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG22 | 3 | 0.11 |
| (1,1714) | 1:103:A:ILE:HG23 | 1:123:A:ILE:HG23 | 3 | 0.11 |
| (1,1689) | 1:90:A:THR:H | 1:103:A:ILE:HB | 3 | 0.11 |
| (1,1676) | 1:102:A:THR:HG21 | 1:103:A:ILE:H | 7 | 0.11 |
| (1,1676) | 1:102:A:THR:HG22 | 1:103:A:ILE:H | 7 | 0.11 |
| (1,1676) | 1:102:A:THR:HG23 | 1:103:A:ILE:H | 7 | 0.11 |
| (1,1655) | 1:94:A:ILE:HG21 | 1:101:A:ALA:HA | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1655) | 1:94:A:ILE:HG22 | 1:101:A:ALA:HA | 8 | 0.11 |
| (1,1655) | 1:94:A:ILE:HG23 | 1:101:A:ALA:HA | 8 | 0.11 |
| (1,1632) | 1:100:A:SER:HA | 1:101:A:ALA:H | 10 | 0.11 |
| (1,1613) | 1:98:A:THR:HA | 1:98:A:THR:HB | 3 | 0.11 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 6 | 0.11 |
| (1,1458) | 1:88:A:GLU:H | 1:87:A:ASN:HB2 | 8 | 0.11 |
| (1,1319) | 1:125:A:LYS:HA | 1:77:A:ILE:HG21 | 10 | 0.11 |
| (1,1319) | 1:125:A:LYS:HA | 1:77:A:ILE:HG22 | 10 | 0.11 |
| (1,1319) | 1:125:A:LYS:HA | 1:77:A:ILE:HG23 | 10 | 0.11 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD11 | 7 | 0.11 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD12 | 7 | 0.11 |
| (1,1303) | 1:78:A:LEU:H | 1:77:A:ILE:HD13 | 7 | 0.11 |
| (1,1269) | 1:91:A:LEU:H | 1:76:A:ARG:HA | 6 | 0.11 |
| (1,1062) | 1:65:A:HIS:HB3 | 1:61:A:LEU:HB2 | 1 | 0.11 |
| (1,1021) | 1:15:A:LEU:HD11 | 1:63:A:GLN:HB2 | 9 | 0.11 |
| (1,1021) | 1:15:A:LEU:HD12 | 1:63:A:GLN:HB2 | 9 | 0.11 |
| (1,1021) | 1:15:A:LEU:HD13 | 1:63:A:GLN:HB2 | 9 | 0.11 |
| (1,951) | 1:60:A:LYS:HA | 1:50:A:VAL:H | 9 | 0.11 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 2 | 0.11 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 2 | 0.11 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 2 | 0.11 |
| (1,886) | 1:54:A:ASP:HA | 1:54:A:ASP:H | 4 | 0.11 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE1 | 8 | 0.11 |
| (1,869) | 1:94:A:ILE:HD11 | 1:120:A:TYR:HE2 | 8 | 0.11 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE1 | 8 | 0.11 |
| (1,869) | 1:94:A:ILE:HD12 | 1:120:A:TYR:HE2 | 8 | 0.11 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE1 | 8 | 0.11 |
| (1,869) | 1:94:A:ILE:HD13 | 1:120:A:TYR:HE2 | 8 | 0.11 |
| (1,861) | 1:53:A:ILE:HD11 | 1:36:A:LYS:HE3 | 4 | 0.11 |
| (1,861) | 1:53:A:ILE:HD12 | 1:36:A:LYS:HE3 | 4 | 0.11 |
| (1,861) | 1:53:A:ILE:HD13 | 1:36:A:LYS:HE3 | 4 | 0.11 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD11 | 1 | 0.11 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD12 | 1 | 0.11 |
| (1,859) | 1:37:A:ALA:HA | 1:53:A:ILE:HD13 | 1 | 0.11 |
| (1,842) | 1:53:A:ILE:HA | 1:53:A:ILE:HG13 | 4 | 0.11 |
| (1,788) | 1:49:A:VAL:HG21 | 1:48:A:ALA:HA | 2 | 0.11 |
| (1,788) | 1:49:A:VAL:HG22 | 1:48:A:ALA:HA | 2 | 0.11 |
| (1,788) | 1:49:A:VAL:HG23 | 1:48:A:ALA:HA | 2 | 0.11 |
| (1,787) | 1:49:A:VAL:HG11 | 1:58:A:LYS:HG2 | 2 | 0.11 |
| (1,787) | 1:49:A:VAL:HG12 | 1:58:A:LYS:HG2 | 2 | 0.11 |
| (1,787) | 1:49:A:VAL:HG13 | 1:58:A:LYS:HG2 | 2 | 0.11 |
| (1,777) | 1:48:A:ALA:HB1 | 1:41:A:GLU:H | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,777) | 1:48:A:ALA:HB2 | 1:41:A:GLU:H | 3 | 0.11 |
| (1,777) | 1:48:A:ALA:HB3 | 1:41:A:GLU:H | 3 | 0.11 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 2 | 0.11 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 2 | 0.11 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 2 | 0.11 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG21 | 4 | 0.11 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG22 | 4 | 0.11 |
| (1,763) | 1:47:A:THR:HB | 1:43:A:ILE:HG23 | 4 | 0.11 |
| (1,747) | 1:46:A:TYR:HA | 1:46:A:TYR:HD1 | 5 | 0.11 |
| (1,747) | 1:46:A:TYR:HA | 1:46:A:TYR:HD2 | 5 | 0.11 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG21 | 5 | 0.11 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG22 | 5 | 0.11 |
| (1,660) | 1:15:A:LEU:H | 1:42:A:VAL:HG23 | 5 | 0.11 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG11 | 4 | 0.11 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG12 | 4 | 0.11 |
| (1,654) | 1:15:A:LEU:HB2 | 1:42:A:VAL:HG13 | 4 | 0.11 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 10 | 0.11 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 3 | 0.11 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 3 | 0.11 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 3 | 0.11 |
| (1,563) | 1:39:A:VAL:HG21 | 1:19:A:ILE:H | 6 | 0.11 |
| (1,563) | 1:39:A:VAL:HG22 | 1:19:A:ILE:H | 6 | 0.11 |
| (1,563) | 1:39:A:VAL:HG23 | 1:19:A:ILE:H | 6 | 0.11 |
| (1,548) | 1:39:A:VAL:HA | 1:50:A:VAL:HB | 6 | 0.11 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 4 | 0.11 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 5 | 0.11 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 9 | 0.11 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 2 | 0.11 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 6 | 0.11 |
| (1,458) | 1:61:A:LEU:HD21 | 1:60:A:LYS:H | 5 | 0.11 |
| (1,458) | 1:61:A:LEU:HD22 | 1:60:A:LYS:H | 5 | 0.11 |
| (1,458) | 1:61:A:LEU:HD23 | 1:60:A:LYS:H | 5 | 0.11 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD11 | 1 | 0.11 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD12 | 1 | 0.11 |
| (1,453) | 1:32:A:TYR:HD1 | 1:28:A:LEU:HD13 | 1 | 0.11 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD11 | 1 | 0.11 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD12 | 1 | 0.11 |
| (1,453) | 1:32:A:TYR:HD2 | 1:28:A:LEU:HD13 | 1 | 0.11 |
| (1,439) | 1:60:A:LYS:HD2 | 1:60:A:LYS:HA | 9 | 0.11 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG21 | 10 | 0.11 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG22 | 10 | 0.11 |
| (1,401) | 1:23:A:ILE:HA | 1:24:A:ILE:HG23 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 5 | 0.11 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 5 | 0.11 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 5 | 0.11 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG21 | 9 | 0.11 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG22 | 9 | 0.11 |
| (1,399) | 1:66:A:LEU:HA | 1:24:A:ILE:HG23 | 9 | 0.11 |
| (1,374) | 1:23:A:ILE:HG21 | 1:33:A:HIS:HD2 | 5 | 0.11 |
| (1,374) | 1:23:A:ILE:HG22 | 1:33:A:HIS:HD2 | 5 | 0.11 |
| (1,374) | 1:23:A:ILE:HG23 | 1:33:A:HIS:HD2 | 5 | 0.11 |
| (1,374) | 1:23:A:ILE:HG21 | 1:33:A:HIS:HD2 | 9 | 0.11 |
| (1,374) | 1:23:A:ILE:HG22 | 1:33:A:HIS:HD2 | 9 | 0.11 |
| (1,374) | 1:23:A:ILE:HG23 | 1:33:A:HIS:HD2 | 9 | 0.11 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 5 | 0.11 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 5 | 0.11 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 5 | 0.11 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 8 | 0.11 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 8 | 0.11 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 8 | 0.11 |
| (1,288) | 1:20:A:ILE:H | 1:20:A:ILE:HG12 | 1 | 0.11 |
| (1,288) | 1:20:A:ILE:H | 1:20:A:ILE:HG12 | 6 | 0.11 |
| (1,288) | 1:20:A:ILE:H | 1:20:A:ILE:HG12 | 7 | 0.11 |
| (1,281) | 1:20:A:ILE:HD11 | 1:20:A:ILE:HB | 4 | 0.11 |
| (1,281) | 1:20:A:ILE:HD12 | 1:20:A:ILE:HB | 4 | 0.11 |
| (1,281) | 1:20:A:ILE:HD13 | 1:20:A:ILE:HB | 4 | 0.11 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 3 | 0.11 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 5 | 0.11 |
| (1,205) | 1:17:A:PRO:HA | 1:17:A:PRO:HG2 | 10 | 0.11 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 8 | 0.11 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 8 | 0.11 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 8 | 0.11 |
| (1,102) | 1:14:A:TRP:HB3 | 1:14:A:TRP:HE3 | 10 | 0.11 |
| (1,81) | 1:47:A:THR:HG21 | 1:60:A:LYS:HE3 | 1 | 0.11 |
| (1,81) | 1:47:A:THR:HG22 | 1:60:A:LYS:HE3 | 1 | 0.11 |
| (1,81) | 1:47:A:THR:HG23 | 1:60:A:LYS:HE3 | 1 | 0.11 |
| (1,28) | 1:7:A:ARG:HB3 | 1:7:A:ARG:HG2 | 6 | 0.11 |
| (1,1) | 1:107:A:THR:HB | 1:108:A:GLY:H | 8 | 0.11 |
| (3,1226) | 1:93:A:SER:H | 1:92:A:GLU:HG2 | 8 | 0.1 |
| (3,1182) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 5 | 0.1 |
| (3,1182) | 1:98:A:THR:HG21 | 1:98:A:THR:HA | 9 | 0.1 |
| (3,1153) | 1:3:A:GLU:HA | 1:4:A:GLU:H | 7 | 0.1 |
| (3,1128) | 1:75:A:LYS:HG2 | 1:72:A:ALA:H | 3 | 0.1 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 4 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 8 | 0.1 |
| (3,1061) | 1:10:A:ARG:HB2 | 1:10:A:ARG:HA | 9 | 0.1 |
| (3,1001) | 1:50:A:VAL:HA | 1:50:A:VAL:H | 7 | 0.1 |
| (3,899) | 1:35:A:LYS:HA | 1:35:A:LYS:H | 8 | 0.1 |
| (3,792) | 1:126:A:LEU:HG | 1:126:A:LEU:HD21 | 5 | 0.1 |
| (3,729) | 1:26:A:LYS:HE2 | 1:26:A:LYS:HD3 | 1 | 0.1 |
| (3,729) | 1:26:A:LYS:HD2 | 1:26:A:LYS:HE3 | 6 | 0.1 |
| (3,646) | 1:85:A:ARG:H | 1:83:A:GLY:H | 1 | 0.1 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 4 | 0.1 |
| (3,481) | 1:93:A:SER:H | 1:93:A:SER:HB3 | 10 | 0.1 |
| (3,450) | 1:103:A:ILE:HG23 | 1:102:A:THR:HA | 1 | 0.1 |
| (3,396) | 1:118:A:ILE:HG23 | 1:121:A:GLU:HA | 8 | 0.1 |
| (3,332) | 1:43:A:ILE:HG21 | 1:43:A:ILE:HG13 | 4 | 0.1 |
| (3,310) | 1:51:A:LYS:HD2 | 1:51:A:LYS:HG3 | 6 | 0.1 |
| (3,296) | 1:91:A:LEU:HD23 | 1:101:A:ALA:HB2 | 5 | 0.1 |
| (3,144) | 1:96:A:GLU:HB2 | 1:97:A:LYS:H | 3 | 0.1 |
| (3,129) | 1:77:A:ILE:HD13 | 1:123:A:ILE:HB | 6 | 0.1 |
| (3,129) | 1:77:A:ILE:HD13 | 1:123:A:ILE:HB | 8 | 0.1 |
| (3,98) | 1:96:A:GLU:HB3 | 1:96:A:GLU:HB2 | 1 | 0.1 |
| (3,98) | 1:2:A:GLU:HB2 | 1:2:A:GLU:HB3 | 2 | 0.1 |
| (3,98) | 1:2:A:GLU:HB2 | 1:2:A:GLU:HB3 | 3 | 0.1 |
| (3,98) | 1:3:A:GLU:HB3 | 1:3:A:GLU:HB2 | 4 | 0.1 |
| (3,98) | 1:2:A:GLU:HB2 | 1:2:A:GLU:HB3 | 5 | 0.1 |
| (3,98) | 1:3:A:GLU:HB3 | 1:3:A:GLU:HB2 | 6 | 0.1 |
| (3,98) | 1:2:A:GLU:HB2 | 1:2:A:GLU:HB3 | 7 | 0.1 |
| (3,98) | 1:3:A:GLU:HB3 | 1:3:A:GLU:HB2 | 8 | 0.1 |
| (3,98) | 1:96:A:GLU:HB3 | 1:96:A:GLU:HB2 | 9 | 0.1 |
| (3,98) | 1:2:A:GLU:HB2 | 1:2:A:GLU:HB3 | 10 | 0.1 |
| (2,650) | 1:61:A:LEU:HB2 | 1:65:A:HIS:HD2 | 4 | 0.1 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG11 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG12 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG21 | 1:115:A:VAL:HG13 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG11 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG12 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG22 | 1:115:A:VAL:HG13 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG11 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG12 | 10 | 0.1 |
| (2,229) | 1:104:A:VAL:HG23 | 1:115:A:VAL:HG13 | 10 | 0.1 |
| (2,61) | 1:26:A:LYS:HE2 | 1:24:A:ILE:HA | 2 | 0.1 |
| (1,3752) | 1:34:A:LYS:HG2 | 1:33:A:HIS:HE1 | 6 | 0.1 |
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 1 | 0.1 |
| (1,3750) | 1:14:A:TRP:HZ2 | 1:63:A:GLN:HB3 | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3737) | 1:5:A:LYS:H | 1:3:A:GLU:H | 10 | 0.1 |
| (1,3710) | 1:82:A:GLY:H | 1:85:A:ARG:HA | 3 | 0.1 |
| (1,3635) | 1:64:A:THR:H | 1:62:A:ASP:H | 8 | 0.1 |
| (1,3575) | 1:87:A:ASN:H | 1:87:A:ASN:HD22 | 5 | 0.1 |
| (1,3557) | 1:10:A:ARG:HG2 | 1:81:A:ASN:HD21 | 9 | 0.1 |
| (1,3547) | 1:84:A:TYR:HB2 | 1:79:A:VAL:H | 8 | 0.1 |
| (1,3544) | 1:66:A:LEU:HD11 | 1:65:A:HIS:H | 3 | 0.1 |
| (1,3544) | 1:66:A:LEU:HD12 | 1:65:A:HIS:H | 3 | 0.1 |
| (1,3544) | 1:66:A:LEU:HD13 | 1:65:A:HIS:H | 3 | 0.1 |
| (1,3449) | 1:15:A:LEU:H | 1:14:A:TRP:HE1 | 5 | 0.1 |
| (1,3317) | 1:22:A:LYS:H | 1:66:A:LEU:HA | 10 | 0.1 |
| (1,3225) | 1:35:A:LYS:H | 1:34:A:LYS:HG3 | 5 | 0.1 |
| (1,3213) | 1:36:A:LYS:H | 1:35:A:LYS:H | 8 | 0.1 |
| (1,3176) | 1:51:A:LYS:HB3 | 1:40:A:LYS:H | 7 | 0.1 |
| (1,3134) | 1:44:A:ASP:H | 1:43:A:ILE:HG13 | 1 | 0.1 |
| (1,3108) | 1:46:A:TYR:H | 1:47:A:THR:HA | 3 | 0.1 |
| (1,2996) | 1:60:A:LYS:HB2 | 1:60:A:LYS:H | 7 | 0.1 |
| (1,2967) | 1:46:A:TYR:HB2 | 1:63:A:GLN:H | 10 | 0.1 |
| (1,2958) | 1:64:A:THR:H | 1:63:A:GLN:HB2 | 7 | 0.1 |
| (1,2865) | 1:75:A:LYS:H | 1:71:A:PRO:HB2 | 5 | 0.1 |
| (1,2786) | 1:81:A:ASN:H | 1:86:A:GLY:H | 4 | 0.1 |
| (1,2636) | 1:96:A:GLU:H | 1:97:A:LYS:HD3 | 9 | 0.1 |
| (1,2634) | 1:96:A:GLU:HG3 | 1:96:A:GLU:H | 7 | 0.1 |
| (1,2607) | 1:97:A:LYS:HG2 | 1:98:A:THR:H | 1 | 0.1 |
| (1,2589) | 1:95:A:ASN:HB3 | 1:100:A:SER:H | 7 | 0.1 |
| (1,2509) | 1:107:A:THR:H | 1:88:A:GLU:H | 3 | 0.1 |
| (1,2509) | 1:107:A:THR:H | 1:88:A:GLU:H | 7 | 0.1 |
| (1,2481) | 1:106:A:GLU:HA | 1:111:A:LYS:H | 9 | 0.1 |
| (1,2454) | 1:113:A:ARG:HD2 | 1:114:A:ARG:H | 9 | 0.1 |
| (1,2336) | 1:77:A:ILE:HA | 1:125:A:LYS:H | 1 | 0.1 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 2 | 0.1 |
| (1,2330) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 10 | 0.1 |
| (1,2252) | 1:40:A:LYS:HE3 | 1:40:A:LYS:HG3 | 2 | 0.1 |
| (1,2193) | 1:107:A:THR:HG21 | 1:87:A:ASN:HA | 3 | 0.1 |
| (1,2193) | 1:107:A:THR:HG22 | 1:87:A:ASN:HA | 3 | 0.1 |
| (1,2193) | 1:107:A:THR:HG23 | 1:87:A:ASN:HA | 3 | 0.1 |
| (1,2178) | 1:104:A:VAL:HG21 | 1:112:A:GLY:HA3 | 10 | 0.1 |
| (1,2178) | 1:104:A:VAL:HG22 | 1:112:A:GLY:HA3 | 10 | 0.1 |
| (1,2178) | 1:104:A:VAL:HG23 | 1:112:A:GLY:HA3 | 10 | 0.1 |
| (1,2149) | 1:118:A:ILE:HG13 | 1:118:A:ILE:HA | 7 | 0.1 |
| (1,2034) | 1:98:A:THR:HG21 | 1:95:A:ASN:HB3 | 10 | 0.1 |
| (1,2034) | 1:98:A:THR:HG22 | 1:95:A:ASN:HB3 | 10 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2034) | 1:98:A:THR:HG23 | 1:95:A:ASN:HB3 | 10 | 0.1 |
| (1,1947) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HA | 7 | 0.1 |
| (1,1946) | 1:117:A:GLY:HA3 | 1:116:A:GLU:HB3 | 7 | 0.1 |
| (1,1788) | 1:107:A:THR:HG21 | 1:107:A:THR:H | 1 | 0.1 |
| (1,1788) | 1:107:A:THR:HG22 | 1:107:A:THR:H | 1 | 0.1 |
| (1,1788) | 1:107:A:THR:HG23 | 1:107:A:THR:H | 1 | 0.1 |
| (1,1785) | 1:107:A:THR:HB | 1:107:A:THR:HA | 7 | 0.1 |
| (1,1785) | 1:107:A:THR:HB | 1:107:A:THR:HA | 9 | 0.1 |
| (1,1667) | 1:102:A:THR:HA | 1:116:A:GLU:HG2 | 4 | 0.1 |
| (1,1492) | 1:104:A:VAL:H | 1:90:A:THR:HB | 8 | 0.1 |
| (1,1441) | 1:85:A:ARG:HB3 | 1:86:A:GLY:H | 2 | 0.1 |
| (1,1396) | 1:122:A:ASP:HA | 1:81:A:ASN:HB3 | 9 | 0.1 |
| (1,1212) | 1:71:A:PRO:HA | 1:72:A:ALA:HA | 2 | 0.1 |
| (1,1087) | 1:21:A:VAL:HB | 1:66:A:LEU:HB2 | 10 | 0.1 |
| (1,941) | 1:59:A:LEU:HD11 | 1:32:A:TYR:HE1 | 5 | 0.1 |
| (1,941) | 1:59:A:LEU:HD11 | 1:32:A:TYR:HE2 | 5 | 0.1 |
| (1,941) | 1:59:A:LEU:HD12 | 1:32:A:TYR:HE1 | 5 | 0.1 |
| (1,941) | 1:59:A:LEU:HD12 | 1:32:A:TYR:HE2 | 5 | 0.1 |
| (1,941) | 1:59:A:LEU:HD13 | 1:32:A:TYR:HE1 | 5 | 0.1 |
| (1,941) | 1:59:A:LEU:HD13 | 1:32:A:TYR:HE2 | 5 | 0.1 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD11 | 4 | 0.1 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD12 | 4 | 0.1 |
| (1,940) | 1:61:A:LEU:HG | 1:59:A:LEU:HD13 | 4 | 0.1 |
| (1,926) | 1:58:A:LYS:HG3 | 1:59:A:LEU:H | 1 | 0.1 |
| (1,922) | 1:60:A:LYS:HE2 | 1:60:A:LYS:HA | 5 | 0.1 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD11 | 1 | 0.1 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD12 | 1 | 0.1 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD13 | 1 | 0.1 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD11 | 9 | 0.1 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD12 | 9 | 0.1 |
| (1,862) | 1:53:A:ILE:HB | 1:53:A:ILE:HD13 | 9 | 0.1 |
| (1,839) | 1:53:A:ILE:HA | 1:53:A:ILE:HG21 | 4 | 0.1 |
| (1,839) | 1:53:A:ILE:HA | 1:53:A:ILE:HG22 | 4 | 0.1 |
| (1,839) | 1:53:A:ILE:HA | 1:53:A:ILE:HG23 | 4 | 0.1 |
| (1,693) | 1:80:A:LEU:HD11 | 1:124:A:SER:HB2 | 2 | 0.1 |
| (1,693) | 1:80:A:LEU:HD12 | 1:124:A:SER:HB2 | 2 | 0.1 |
| (1,693) | 1:80:A:LEU:HD13 | 1:124:A:SER:HB2 | 2 | 0.1 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG21 | 10 | 0.1 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG22 | 10 | 0.1 |
| (1,659) | 1:45:A:LYS:H | 1:42:A:VAL:HG23 | 10 | 0.1 |
| (1,632) | 1:41:A:GLU:HB3 | 1:41:A:GLU:HG2 | 9 | 0.1 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD11 | 10 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD12 | 10 | 0.1 |
| (1,585) | 1:127:A:ALA:HA | 1:38:A:ILE:HD13 | 10 | 0.1 |
| (1,478) | 1:31:A:LYS:HB3 | 1:31:A:LYS:HA | 2 | 0.1 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 1 | 0.1 |
| (1,468) | 1:30:A:GLU:HB3 | 1:30:A:GLU:HA | 5 | 0.1 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG21 | 9 | 0.1 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG22 | 9 | 0.1 |
| (1,400) | 1:24:A:ILE:HA | 1:24:A:ILE:HG23 | 9 | 0.1 |
| (1,309) | 1:21:A:VAL:HG21 | 1:14:A:TRP:HH2 | 3 | 0.1 |
| (1,309) | 1:21:A:VAL:HG22 | 1:14:A:TRP:HH2 | 3 | 0.1 |
| (1,309) | 1:21:A:VAL:HG23 | 1:14:A:TRP:HH2 | 3 | 0.1 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD21 | 1 | 0.1 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD22 | 1 | 0.1 |
| (1,150) | 1:48:A:ALA:H | 1:15:A:LEU:HD23 | 1 | 0.1 |
| (1,148) | 1:15:A:LEU:HD11 | 1:14:A:TRP:HZ2 | 9 | 0.1 |
| (1,148) | 1:15:A:LEU:HD12 | 1:14:A:TRP:HZ2 | 9 | 0.1 |
| (1,148) | 1:15:A:LEU:HD13 | 1:14:A:TRP:HZ2 | 9 | 0.1 |
| (1,52) | 1:61:A:LEU:HD11 | 1:25:A:THR:HB | 5 | 0.1 |
| (1,52) | 1:61:A:LEU:HD12 | 1:25:A:THR:HB | 5 | 0.1 |
| (1,52) | 1:61:A:LEU:HD13 | 1:25:A:THR:HB | 5 | 0.1 |
| (1,28) | 1:7:A:ARG:HB2 | 1:7:A:ARG:HG3 | 2 | 0.1 |
| (1,28) | 1:7:A:ARG:HB2 | 1:7:A:ARG:HG3 | 5 | 0.1 |
| (1,14) | 1:5:A:LYS:HA | 1:5:A:LYS:HD2 | 8 | 0.1 |

10 Dihedral-angle violation analysis

No dihedral-angle restraints found