



Full wwPDB NMR Structure Validation Report ⓘ

Jun 21, 2026 – 01:15 pm BST

PDB ID : 9T3O / pdb_00009t3o
BMRB ID : 35025
Title : Solution structure of thanatin in complex with LptDm
Authors : Schuster, M.; Zerbe, O.
Deposited on : 2025-10-28

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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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

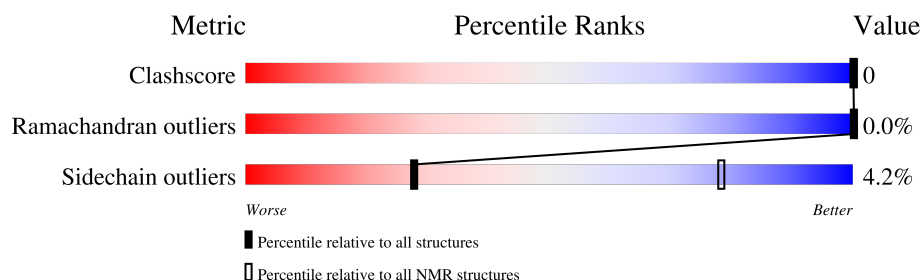
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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 | 229148 | 14424 |
| Ramachandran outliers | 224038 | 12848 |
| Sidechain outliers | 223484 | 12823 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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 | 181 | |
| 2 | B | 21 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:51-A:90, A:101-A:224, B:8-B:21 (178) | 0.63 | 11 |

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3045 atoms, of which 1518 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LPS-assembly protein LptD.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1 | A | 181 | Total | C | H | N | O | S | 0 |
| | | | 2694 | 847 | 1335 | 229 | 281 | 2 | |

There are 93 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 133 | TRP | - | expression tag | UNP P31554 |
| A | 134 | VAL | - | expression tag | UNP P31554 |
| A | 135 | PHE | - | expression tag | UNP P31554 |
| A | 136 | TYR | - | expression tag | UNP P31554 |
| A | 137 | ASP | - | expression tag | UNP P31554 |
| A | 138 | ALA | - | expression tag | UNP P31554 |
| A | 139 | SER | - | expression tag | UNP P31554 |
| A | 140 | ILE | - | expression tag | UNP P31554 |
| A | 141 | GLU | - | expression tag | UNP P31554 |
| A | 142 | THR | - | expression tag | UNP P31554 |
| A | 143 | VAL | - | expression tag | UNP P31554 |
| A | 144 | GLY | - | expression tag | UNP P31554 |
| A | 145 | ALA | - | expression tag | UNP P31554 |
| A | 146 | PRO | - | expression tag | UNP P31554 |
| A | 147 | GLY | - | expression tag | UNP P31554 |
| A | 148 | SER | - | expression tag | UNP P31554 |
| A | 149 | ALA | - | expression tag | UNP P31554 |
| A | 150 | SER | - | expression tag | UNP P31554 |
| A | 151 | ALA | - | expression tag | UNP P31554 |
| A | 152 | LYS | - | expression tag | UNP P31554 |
| A | 153 | VAL | - | expression tag | UNP P31554 |
| A | 154 | ILE | - | expression tag | UNP P31554 |
| A | 155 | LYS | - | expression tag | UNP P31554 |
| A | 156 | SER | - | expression tag | UNP P31554 |
| A | 157 | LEU | - | expression tag | UNP P31554 |
| A | 158 | ASP | - | expression tag | UNP P31554 |
| A | 159 | ASN | - | expression tag | UNP P31554 |
| A | 160 | GLY | - | expression tag | UNP P31554 |
| A | 161 | LYS | - | expression tag | UNP P31554 |
| A | 162 | THR | - | expression tag | UNP P31554 |
| A | 163 | LEU | - | expression tag | UNP P31554 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 164 | GLU | - | expression tag | UNP P31554 |
| A | 165 | PHE | - | expression tag | UNP P31554 |
| A | 166 | ASP | - | expression tag | UNP P31554 |
| A | 167 | ASP | - | expression tag | UNP P31554 |
| A | 168 | ALA | - | expression tag | UNP P31554 |
| A | 169 | THR | - | expression tag | UNP P31554 |
| A | 170 | PHE | - | expression tag | UNP P31554 |
| A | 171 | ASP | - | expression tag | UNP P31554 |
| A | 172 | SER | - | expression tag | UNP P31554 |
| A | 173 | TYR | - | expression tag | UNP P31554 |
| A | 174 | GLU | - | expression tag | UNP P31554 |
| A | 175 | ASN | - | expression tag | UNP P31554 |
| A | 176 | ALA | - | expression tag | UNP P31554 |
| A | 177 | GLU | - | expression tag | UNP P31554 |
| A | 178 | ALA | - | expression tag | UNP P31554 |
| A | 179 | LEU | - | expression tag | UNP P31554 |
| A | 180 | ILE | - | expression tag | UNP P31554 |
| A | 181 | GLU | - | expression tag | UNP P31554 |
| A | 182 | HIS | - | expression tag | UNP P31554 |
| A | 183 | ALA | - | expression tag | UNP P31554 |
| A | 184 | ILE | - | expression tag | UNP P31554 |
| A | 185 | LYS | - | expression tag | UNP P31554 |
| A | 186 | THR | - | expression tag | UNP P31554 |
| A | 187 | MET | - | expression tag | UNP P31554 |
| A | 188 | GLY | - | expression tag | UNP P31554 |
| A | 189 | VAL | - | expression tag | UNP P31554 |
| A | 190 | LYS | - | expression tag | UNP P31554 |
| A | 191 | THR | - | expression tag | UNP P31554 |
| A | 192 | ILE | - | expression tag | UNP P31554 |
| A | 193 | THR | - | expression tag | UNP P31554 |
| A | 194 | ILE | - | expression tag | UNP P31554 |
| A | 195 | ASN | - | expression tag | UNP P31554 |
| A | 196 | ASN | - | expression tag | UNP P31554 |
| A | 197 | ALA | - | expression tag | UNP P31554 |
| A | 198 | THR | - | expression tag | UNP P31554 |
| A | 199 | GLY | - | expression tag | UNP P31554 |
| A | 200 | ALA | - | expression tag | UNP P31554 |
| A | 201 | ILE | - | expression tag | UNP P31554 |
| A | 202 | THR | - | expression tag | UNP P31554 |
| A | 203 | ALA | - | expression tag | UNP P31554 |
| A | 204 | GLU | - | expression tag | UNP P31554 |
| A | 205 | LYS | - | expression tag | UNP P31554 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 206 | ALA | - | expression tag | UNP P31554 |
| A | 207 | THR | - | expression tag | UNP P31554 |
| A | 208 | LYS | - | expression tag | UNP P31554 |
| A | 209 | LEU | - | expression tag | UNP P31554 |
| A | 210 | LYS | - | expression tag | UNP P31554 |
| A | 211 | ALA | - | expression tag | UNP P31554 |
| A | 212 | LYS | - | expression tag | UNP P31554 |
| A | 213 | ALA | - | expression tag | UNP P31554 |
| A | 214 | ALA | - | expression tag | UNP P31554 |
| A | 215 | GLU | - | expression tag | UNP P31554 |
| A | 216 | LEU | - | expression tag | UNP P31554 |
| A | 217 | GLY | - | expression tag | UNP P31554 |
| A | 218 | ALA | - | expression tag | UNP P31554 |
| A | 219 | THR | - | expression tag | UNP P31554 |
| A | 220 | LEU | - | expression tag | UNP P31554 |
| A | 221 | THR | - | expression tag | UNP P31554 |
| A | 222 | ILE | - | expression tag | UNP P31554 |
| A | 223 | THR | - | expression tag | UNP P31554 |
| A | 224 | LEU | - | expression tag | UNP P31554 |
| A | 225 | LYS | - | expression tag | UNP P31554 |

- Molecule 2 is a protein called Thanatin.

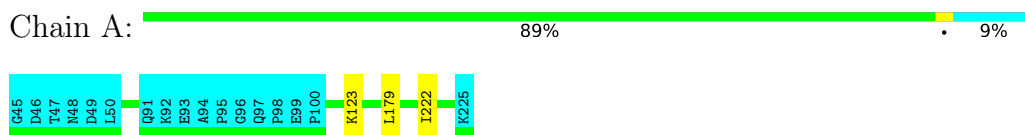
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 2 | B | 21 | Total | C | H | N | O | S | 0 |
| | | | 351 | 103 | 183 | 35 | 27 | 3 | |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: LPS-assembly protein LptD



- Molecule 2: Thanatin

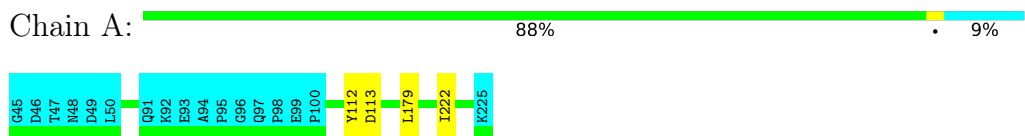


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: LPS-assembly protein LptD

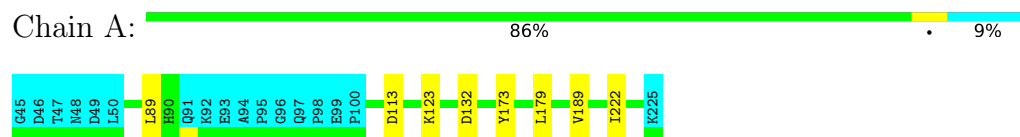


- Molecule 2: Thanatin



4.2.2 Score per residue for model 2

- Molecule 1: LPS-assembly protein LptD

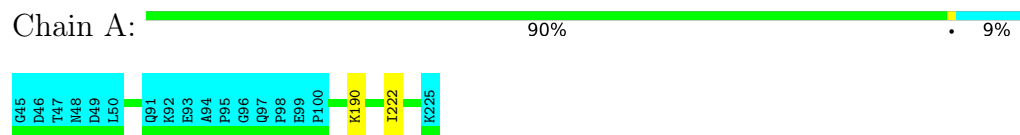


- Molecule 2: Thanatin



4.2.3 Score per residue for model 3

- Molecule 1: LPS-assembly protein LptD

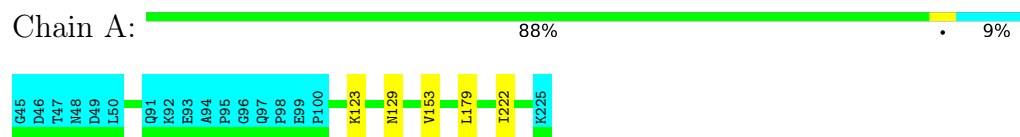


- Molecule 2: Thanatin



4.2.4 Score per residue for model 4

- Molecule 1: LPS-assembly protein LptD

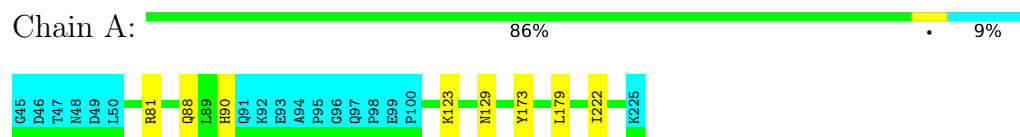


- Molecule 2: Thanatin



4.2.5 Score per residue for model 5

- Molecule 1: LPS-assembly protein LptD

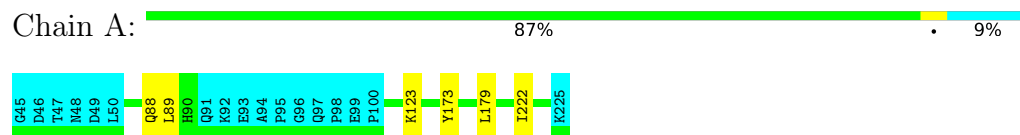


- Molecule 2: Thanatin

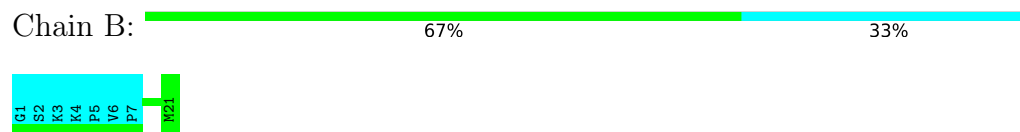


4.2.6 Score per residue for model 6

- Molecule 1: LPS-assembly protein LptD

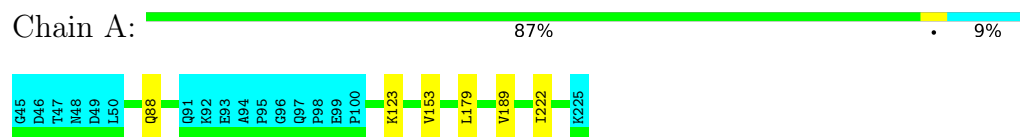


- Molecule 2: Thanatin



4.2.7 Score per residue for model 7

- Molecule 1: LPS-assembly protein LptD

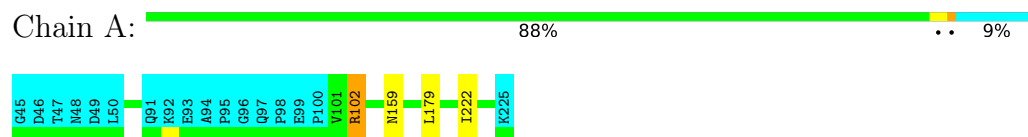


- Molecule 2: Thanatin

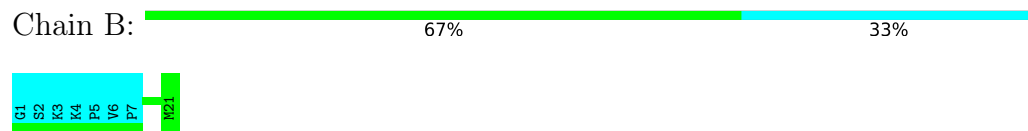


4.2.8 Score per residue for model 8

- Molecule 1: LPS-assembly protein LptD

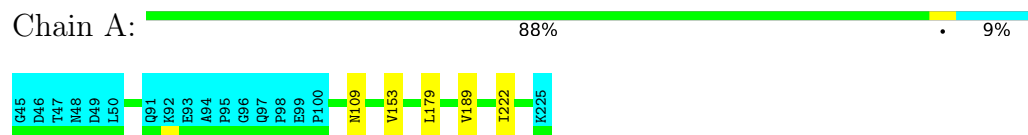


- Molecule 2: Thanatin



4.2.9 Score per residue for model 9

- Molecule 1: LPS-assembly protein LptD

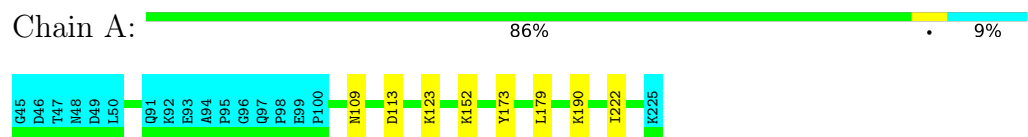


- Molecule 2: Thanatin



4.2.10 Score per residue for model 10

- Molecule 1: LPS-assembly protein LptD

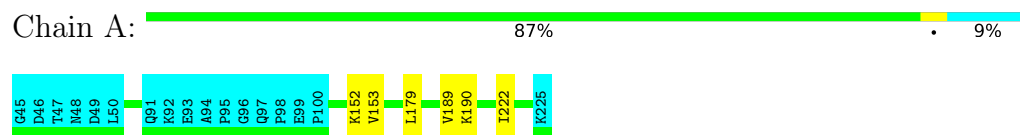


- Molecule 2: Thanatin

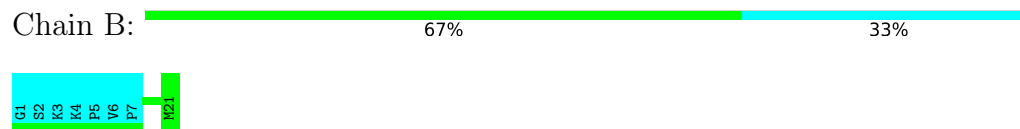


4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: LPS-assembly protein LptD

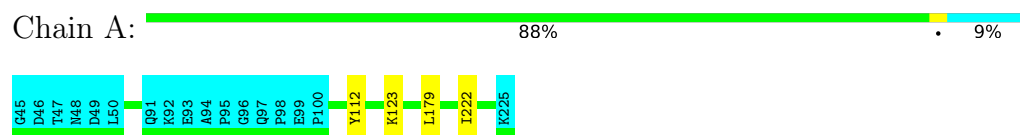


- Molecule 2: Thanatin

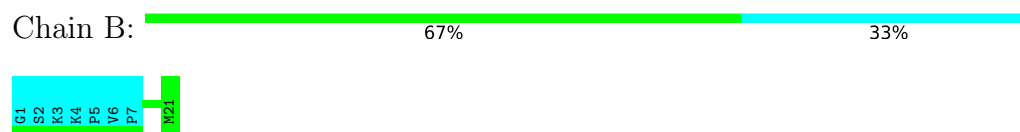


4.2.12 Score per residue for model 12

- Molecule 1: LPS-assembly protein LptD

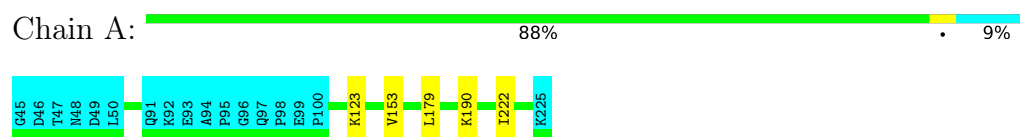


- Molecule 2: Thanatin



4.2.13 Score per residue for model 13

- Molecule 1: LPS-assembly protein LptD

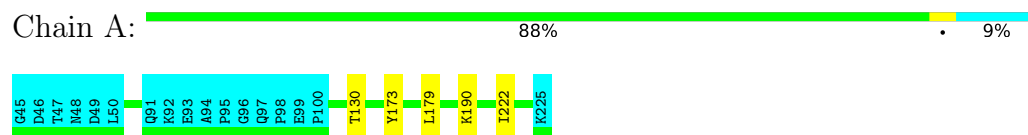


- Molecule 2: Thanatin



4.2.14 Score per residue for model 14

- Molecule 1: LPS-assembly protein LptD

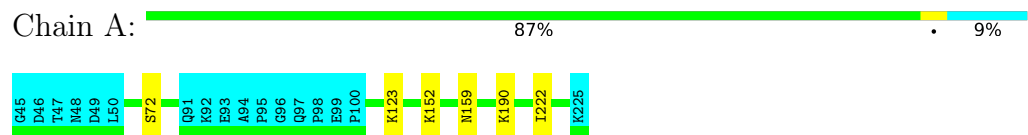


- Molecule 2: Thanatin



4.2.15 Score per residue for model 15

- Molecule 1: LPS-assembly protein LptD

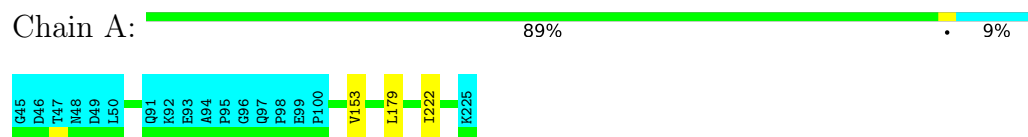


- Molecule 2: Thanatin



4.2.16 Score per residue for model 16

- Molecule 1: LPS-assembly protein LptD

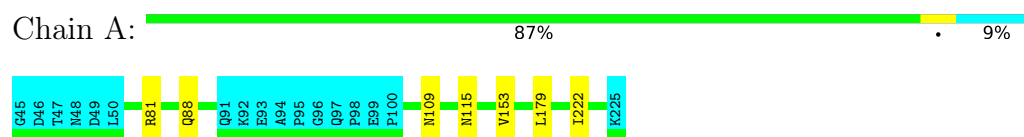


- Molecule 2: Thanatin

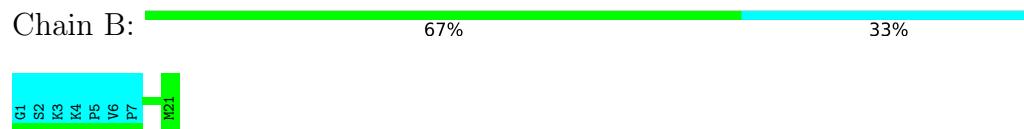


4.2.17 Score per residue for model 17

- Molecule 1: LPS-assembly protein LptD

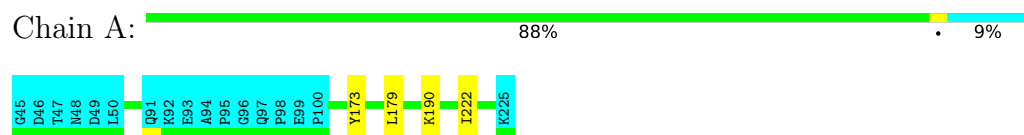


- Molecule 2: Thanatin



4.2.18 Score per residue for model 18

- Molecule 1: LPS-assembly protein LptD

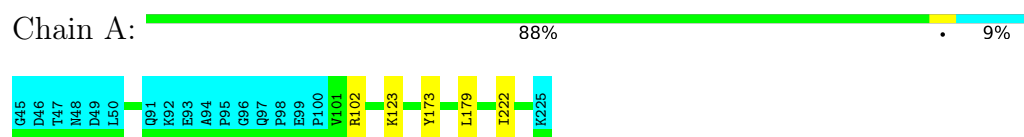


- Molecule 2: Thanatin



4.2.19 Score per residue for model 19

- Molecule 1: LPS-assembly protein LptD




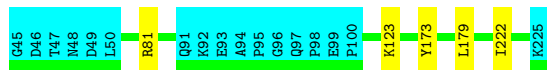
- Molecule 2: Thanatin



4.2.20 Score per residue for model 20

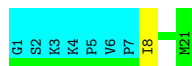
- Molecule 1: LPS-assembly protein LptD

Chain A:  88% 9%



- Molecule 2: Thanatin

Chain B:  62% 5% 33%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| Amber | refinement | Amber19 |
| CYANA | structure calculation | 3.98 |

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 | 2278 |
| Number of shifts mapped to atoms | 2278 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 89% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.84±0.00 | 0±0/1251 (0.0± 0.0%) | 1.37±0.01 | 0±0/1702 (0.0± 0.0%) |
| 2 | B | 0.92±0.01 | 0±0/119 (0.0± 0.0%) | 1.33±0.05 | 0±0/154 (0.0± 0.0%) |
| All | All | 0.85 | 0/27400 (0.0%) | 1.37 | 1/37120 (0.0%) |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 0.1±0.3 |
| All | All | 0 | 2 |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 132 | ASP | CA-CB-CG | 5.02 | 117.62 | 112.60 | 2 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 102 | ARG | Sidechain | 2 |

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 |
|-----|-------|-------|----------|----------|---------|
| All | All | 27000 | 26780 | 26780 | - |

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 -.

There are no clashes.

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 | 164/181 (91%) | 158±2 (96±1%) | 6±2 (4±1%) | 0±0 (0±0%) | 100 | 100 |
| 2 | B | 13/21 (62%) | 13±0 (100±2%) | 0±0 (0±2%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 3540/4040 (88%) | 3421 (97%) | 118 (3%) | 1 (0%) | 100 | 100 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 72 | SER | 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 | 130/144 (90%) | 125±2 (96±1%) | 5±2 (4±1%) | 29 | 79 |
| 2 | B | 13/19 (68%) | 12±1 (93±4%) | 1±1 (7±4%) | 17 | 66 |
| All | All | 2860/3260 (88%) | 2740 (96%) | 120 (4%) | 28 | 78 |

All 22 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 | 222 | ILE | 20 |
| 1 | A | 179 | LEU | 18 |
| 2 | B | 8 | ILE | 13 |
| 1 | A | 123 | LYS | 11 |
| 1 | A | 173 | TYR | 8 |
| 1 | A | 190 | LYS | 7 |
| 1 | A | 153 | VAL | 7 |
| 2 | B | 17 | LYS | 4 |
| 1 | A | 189 | VAL | 4 |
| 1 | A | 88 | GLN | 4 |
| 1 | A | 113 | ASP | 3 |
| 1 | A | 81 | ARG | 3 |
| 1 | A | 109 | ASN | 3 |
| 1 | A | 152 | LYS | 3 |
| 1 | A | 112 | TYR | 2 |
| 1 | A | 89 | LEU | 2 |
| 1 | A | 129 | ASN | 2 |
| 1 | A | 159 | ASN | 2 |
| 1 | A | 90 | HIS | 1 |
| 1 | A | 102 | ARG | 1 |
| 1 | A | 130 | THR | 1 |
| 1 | A | 115 | ASN | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *LptDm-Than*

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 | 2278 |
| Number of shifts mapped to atoms | 2278 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 2 |

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 |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 179 | -0.21 ± 0.10 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 166 | -0.33 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 179 | 0.28 ± 0.08 | None needed (< 0.5 ppm) |
| ^{15}N | 168 | -0.15 ± 0.25 | None needed (< 0.5 ppm) |

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 89%, i.e. 2073 atoms were assigned a chemical shift out of a possible 2320. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone | 846/895 (95%) | 361/365 (99%) | 328/356 (92%) | 157/174 (90%) |
| Sidechain | 1135/1288 (88%) | 800/839 (95%) | 321/404 (79%) | 14/45 (31%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|-----------------|-----------------|-----------------|-----------------|
| Aromatic | 92/137 (67%) | 57/68 (84%) | 35/63 (56%) | 0/6 (0%) |
| Overall | 2073/2320 (89%) | 1218/1272 (96%) | 684/823 (83%) | 171/225 (76%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 2278 atoms were assigned a chemical shift out of a possible 2615. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 920/1008 (91%) | 394/411 (96%) | 358/404 (89%) | 168/193 (87%) |
| Sidechain | 1266/1470 (86%) | 897/954 (94%) | 352/464 (76%) | 17/52 (33%) |
| Aromatic | 92/137 (67%) | 57/68 (84%) | 35/63 (56%) | 0/6 (0%) |
| Overall | 2278/2615 (87%) | 1348/1433 (94%) | 745/931 (80%) | 185/251 (74%) |

7.1.4 Statistically unusual chemical shifts ⓘ

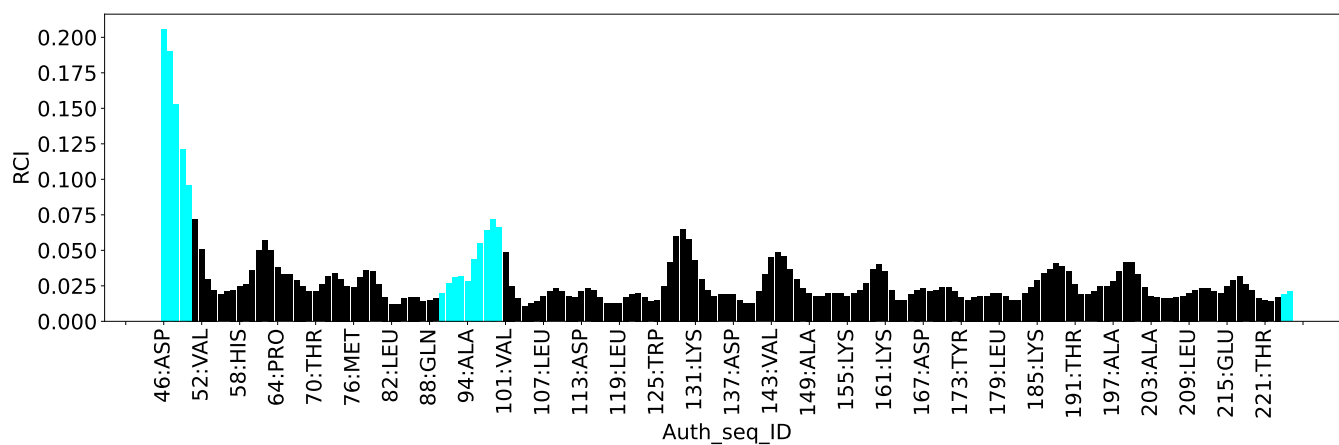
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 156 | SER | HB2 | 1.73 | 2.61 – 5.13 | -8.5 |
| 1 | A | 156 | SER | HB3 | 1.56 | 2.49 – 5.20 | -8.4 |

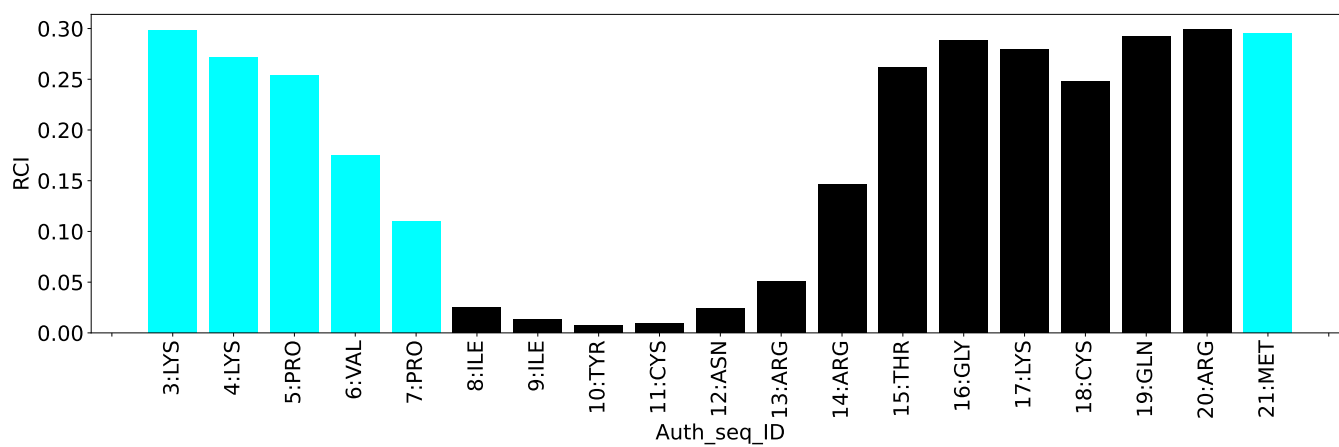
7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



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 | 4051 |
| Intra-residue ($ i-j =0$) | 810 |
| Sequential ($ i-j =1$) | 1113 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 540 |
| Long range ($ i-j \geq 5$) | 1469 |
| Inter-chain | 119 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 20.1 |
| Number of long range restraints per residue ¹ | 7.3 |

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small) | 119.1 | 0.2 |
| 0.2-0.5 (Medium) | 213.8 | 0.5 |
| >0.5 (Large) | 232.7 | 4.9 |

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 ⓘ

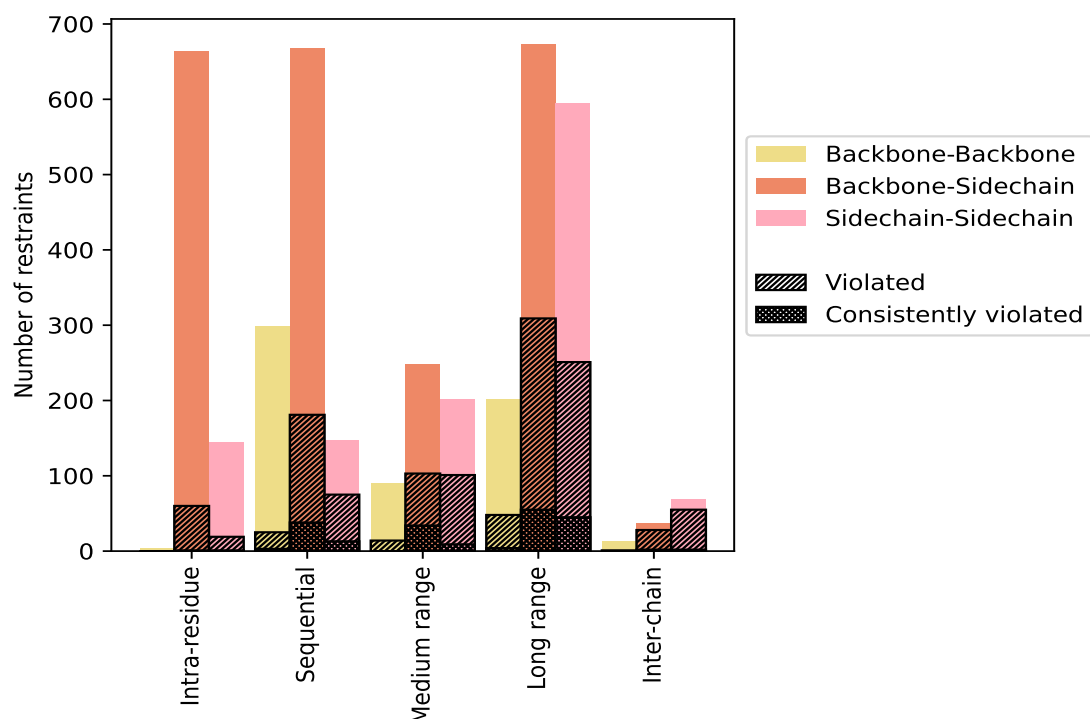
9.1 Summary of distance violations ⓘ

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.

| Restraints type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 810 | 20.0 | 79 | 9.8 | 2.0 | 2 | 0.2 | 0.0 |
| Backbone-Backbone | 3 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 663 | 16.4 | 60 | 9.0 | 1.5 | 1 | 0.2 | 0.0 |
| Sidechain-Sidechain | 144 | 3.6 | 19 | 13.2 | 0.5 | 1 | 0.7 | 0.0 |
| Sequential ($i-j =1$) | 1113 | 27.5 | 281 | 25.2 | 6.9 | 54 | 4.9 | 1.3 |
| Backbone-Backbone | 299 | 7.4 | 25 | 8.4 | 0.6 | 3 | 1.0 | 0.1 |
| Backbone-Sidechain | 667 | 16.5 | 181 | 27.1 | 4.5 | 38 | 5.7 | 0.9 |
| Sidechain-Sidechain | 147 | 3.6 | 75 | 51.0 | 1.9 | 13 | 8.8 | 0.3 |
| Medium range ($i-j >1$ & $i-j <5$) | 540 | 13.3 | 218 | 40.4 | 5.4 | 43 | 8.0 | 1.1 |
| Backbone-Backbone | 90 | 2.2 | 14 | 15.6 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 248 | 6.1 | 103 | 41.5 | 2.5 | 34 | 13.7 | 0.8 |
| Sidechain-Sidechain | 202 | 5.0 | 101 | 50.0 | 2.5 | 9 | 4.5 | 0.2 |
| Long range ($i-j \geq 5$) | 1469 | 36.3 | 608 | 41.4 | 15.0 | 104 | 7.1 | 2.6 |
| Backbone-Backbone | 202 | 5.0 | 48 | 23.8 | 1.2 | 4 | 2.0 | 0.1 |
| Backbone-Sidechain | 673 | 16.6 | 309 | 45.9 | 7.6 | 55 | 8.2 | 1.4 |
| Sidechain-Sidechain | 594 | 14.7 | 251 | 42.3 | 6.2 | 45 | 7.6 | 1.1 |
| Inter-chain | 119 | 2.9 | 84 | 70.6 | 2.1 | 4 | 3.4 | 0.1 |
| Backbone-Backbone | 13 | 0.3 | 1 | 7.7 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 37 | 0.9 | 28 | 75.7 | 0.7 | 2 | 5.4 | 0.0 |
| Sidechain-Sidechain | 69 | 1.7 | 55 | 79.7 | 1.4 | 2 | 2.9 | 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 | 4051 | 100.0 | 1270 | 31.4 | 31.4 | 207 | 5.1 | 5.1 |
| Backbone-Backbone | 607 | 15.0 | 88 | 14.5 | 2.2 | 7 | 1.2 | 0.2 |
| Backbone-Sidechain | 2288 | 56.5 | 681 | 29.8 | 16.8 | 130 | 5.7 | 3.2 |
| Sidechain-Sidechain | 1156 | 28.5 | 501 | 43.3 | 12.4 | 70 | 6.1 | 1.7 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 18 | 139 | 98 | 267 | 37 | 559 | 0.55 | 3.42 | 0.46 | 0.4 |
| 2 | 18 | 134 | 104 | 279 | 32 | 567 | 0.63 | 4.9 | 0.64 | 0.41 |
| 3 | 20 | 150 | 106 | 267 | 43 | 586 | 0.51 | 3.1 | 0.42 | 0.37 |
| 4 | 24 | 138 | 109 | 272 | 32 | 575 | 0.55 | 3.03 | 0.45 | 0.41 |
| 5 | 19 | 134 | 98 | 297 | 40 | 588 | 0.58 | 2.38 | 0.45 | 0.45 |
| 6 | 23 | 130 | 108 | 279 | 28 | 568 | 0.63 | 4.48 | 0.64 | 0.43 |
| 7 | 26 | 137 | 114 | 283 | 33 | 593 | 0.59 | 3.64 | 0.51 | 0.42 |
| 8 | 22 | 140 | 116 | 273 | 26 | 577 | 0.57 | 3.45 | 0.46 | 0.42 |
| 9 | 19 | 137 | 101 | 291 | 29 | 577 | 0.56 | 3.33 | 0.53 | 0.38 |
| 10 | 22 | 133 | 107 | 271 | 31 | 564 | 0.57 | 3.37 | 0.5 | 0.41 |

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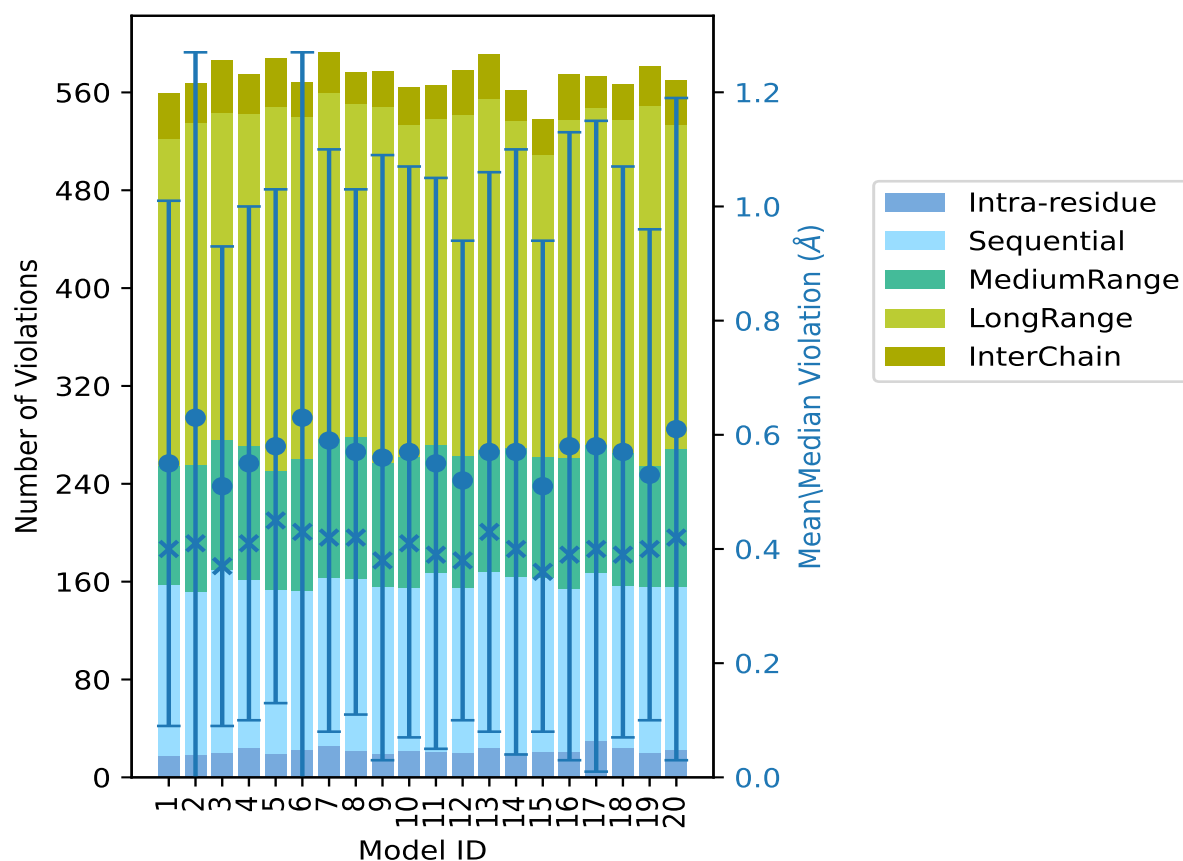
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 21 | 146 | 105 | 267 | 27 | 566 | 0.55 | 4.19 | 0.5 | 0.39 |
| 12 | 20 | 135 | 108 | 279 | 36 | 578 | 0.52 | 2.66 | 0.42 | 0.38 |
| 13 | 24 | 144 | 100 | 287 | 36 | 591 | 0.57 | 3.92 | 0.49 | 0.43 |
| 14 | 20 | 144 | 105 | 268 | 25 | 562 | 0.57 | 4.63 | 0.53 | 0.4 |
| 15 | 21 | 142 | 99 | 247 | 29 | 538 | 0.51 | 3.3 | 0.43 | 0.36 |
| 16 | 21 | 133 | 107 | 277 | 37 | 575 | 0.58 | 4.18 | 0.55 | 0.39 |
| 17 | 30 | 137 | 105 | 275 | 26 | 573 | 0.58 | 4.38 | 0.57 | 0.4 |
| 18 | 24 | 133 | 108 | 273 | 29 | 567 | 0.57 | 3.42 | 0.5 | 0.39 |
| 19 | 20 | 136 | 99 | 294 | 32 | 581 | 0.53 | 3.39 | 0.43 | 0.4 |
| 20 | 22 | 134 | 113 | 265 | 36 | 570 | 0.61 | 4.86 | 0.58 | 0.42 |

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

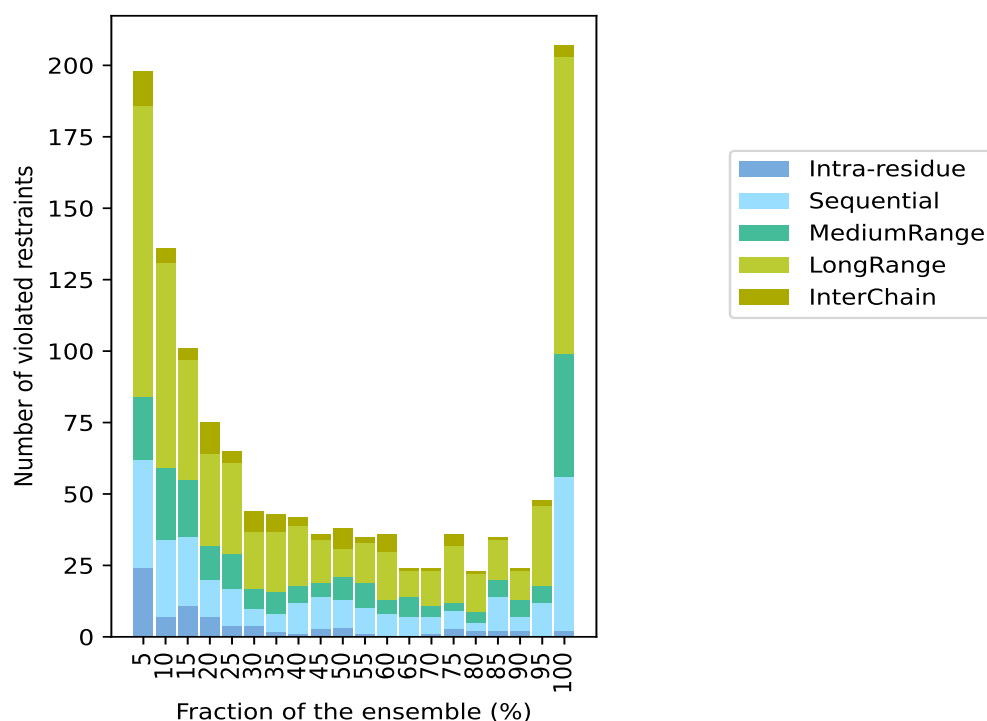
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2781(IR:731, SQ:832, MR:322, LR:861, IC:35) restraints are 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 | % |
| 24 | 38 | 22 | 102 | 12 | 198 | 1 | 5.0 |
| 7 | 27 | 25 | 72 | 5 | 136 | 2 | 10.0 |
| 11 | 24 | 20 | 42 | 4 | 101 | 3 | 15.0 |
| 7 | 13 | 12 | 32 | 11 | 75 | 4 | 20.0 |
| 4 | 13 | 12 | 32 | 4 | 65 | 5 | 25.0 |
| 4 | 6 | 7 | 20 | 7 | 44 | 6 | 30.0 |
| 2 | 6 | 8 | 21 | 6 | 43 | 7 | 35.0 |
| 1 | 11 | 6 | 21 | 3 | 42 | 8 | 40.0 |
| 3 | 11 | 5 | 15 | 2 | 36 | 9 | 45.0 |
| 3 | 10 | 8 | 10 | 7 | 38 | 10 | 50.0 |
| 1 | 9 | 9 | 14 | 2 | 35 | 11 | 55.0 |
| 0 | 8 | 5 | 17 | 6 | 36 | 12 | 60.0 |
| 0 | 7 | 7 | 9 | 1 | 24 | 13 | 65.0 |
| 1 | 6 | 4 | 12 | 1 | 24 | 14 | 70.0 |
| 3 | 6 | 3 | 20 | 4 | 36 | 15 | 75.0 |
| 2 | 3 | 4 | 13 | 1 | 23 | 16 | 80.0 |
| 2 | 12 | 6 | 14 | 1 | 35 | 17 | 85.0 |
| 2 | 5 | 6 | 10 | 1 | 24 | 18 | 90.0 |
| 0 | 12 | 6 | 28 | 2 | 48 | 19 | 95.0 |
| 2 | 54 | 43 | 104 | 4 | 207 | 20 | 100.0 |

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

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

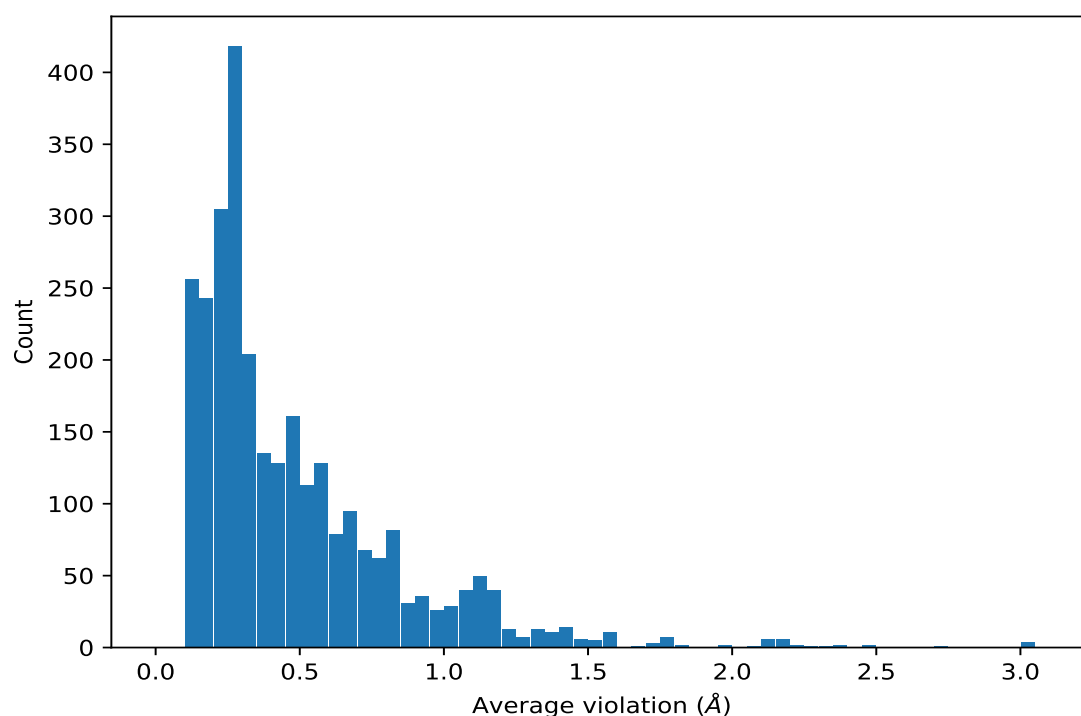
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 20 | 3.02 | 1.27 | 2.87 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 20 | 3.02 | 1.27 | 2.87 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 20 | 3.01 | 0.92 | 2.93 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 20 | 3.01 | 0.92 | 2.93 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 20 | 2.71 | 0.51 | 2.75 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 20 | 2.49 | 1.25 | 2.34 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 20 | 2.49 | 1.25 | 2.34 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 20 | 2.39 | 1.19 | 2.24 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 20 | 2.39 | 1.19 | 2.24 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 20 | 2.33 | 1.29 | 3.14 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 20 | 2.27 | 0.47 | 2.3 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 20 | 2.09 | 0.36 | 1.99 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 20 | 1.8 | 0.31 | 1.8 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 20 | 1.8 | 0.31 | 1.8 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 20 | 1.78 | 0.51 | 1.8 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 20 | 1.75 | 0.33 | 1.9 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 20 | 1.75 | 0.33 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 20 | 1.75 | 0.33 | 1.9 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 20 | 1.74 | 0.5 | 1.99 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 20 | 1.74 | 0.5 | 1.99 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 20 | 1.74 | 0.5 | 1.99 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 20 | 1.58 | 0.24 | 1.56 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 20 | 1.58 | 0.24 | 1.56 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 20 | 1.58 | 0.24 | 1.56 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 20 | 1.58 | 0.24 | 1.56 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 20 | 1.58 | 0.24 | 1.56 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 20 | 1.58 | 0.24 | 1.56 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 20 | 1.57 | 0.22 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 20 | 1.57 | 0.22 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 20 | 1.57 | 0.22 | 1.62 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 20 | 1.54 | 0.39 | 1.53 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 20 | 1.5 | 0.32 | 1.62 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 20 | 1.5 | 0.32 | 1.62 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 20 | 1.5 | 0.32 | 1.62 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 20 | 1.5 | 0.33 | 1.54 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 20 | 1.44 | 0.11 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 20 | 1.44 | 0.11 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 20 | 1.44 | 0.11 | 1.5 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 20 | 1.41 | 0.33 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 20 | 1.41 | 0.33 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 20 | 1.41 | 0.33 | 1.6 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 20 | 1.4 | 0.45 | 1.34 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 20 | 1.4 | 0.45 | 1.34 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 20 | 1.38 | 0.72 | 1.86 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 20 | 1.37 | 0.77 | 1.77 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 20 | 1.36 | 0.3 | 1.36 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 20 | 1.36 | 0.3 | 1.36 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 20 | 1.36 | 0.3 | 1.36 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 20 | 1.34 | 0.54 | 1.31 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 20 | 1.34 | 0.54 | 1.31 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 20 | 1.33 | 0.14 | 1.35 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 20 | 1.33 | 0.08 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 20 | 1.33 | 0.08 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 20 | 1.33 | 0.08 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 20 | 1.33 | 0.08 | 1.36 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 20 | 1.32 | 0.37 | 1.38 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 20 | 1.3 | 0.69 | 1.02 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 20 | 1.27 | 0.36 | 1.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 20 | 1.25 | 0.32 | 1.31 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 20 | 1.25 | 0.32 | 1.31 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 20 | 1.2 | 0.09 | 1.23 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 20 | 1.2 | 0.09 | 1.23 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 20 | 1.2 | 0.09 | 1.23 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 20 | 1.2 | 0.09 | 1.23 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 20 | 1.2 | 0.35 | 1.05 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 20 | 1.2 | 0.35 | 1.05 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 20 | 1.19 | 0.07 | 1.17 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 20 | 1.16 | 0.11 | 1.14 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 20 | 1.16 | 0.11 | 1.14 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 20 | 1.16 | 0.11 | 1.14 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 20 | 1.14 | 0.2 | 1.1 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 20 | 1.14 | 0.2 | 1.1 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 20 | 1.14 | 0.2 | 1.1 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 20 | 1.14 | 0.49 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 20 | 1.14 | 0.49 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 20 | 1.14 | 0.49 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 20 | 1.14 | 0.49 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 20 | 1.14 | 0.49 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 20 | 1.14 | 0.49 | 1.38 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 20 | 1.13 | 0.26 | 1.2 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 20 | 1.13 | 0.26 | 1.2 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 20 | 1.12 | 0.32 | 1.12 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 20 | 1.11 | 0.25 | 1.18 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 20 | 1.11 | 0.25 | 1.18 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 20 | 1.09 | 0.31 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 20 | 1.09 | 0.31 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 20 | 1.09 | 0.31 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 20 | 1.09 | 0.31 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 20 | 1.09 | 0.31 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 20 | 1.09 | 0.31 | 1.1 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 20 | 1.08 | 0.27 | 1.17 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 20 | 1.08 | 0.27 | 1.17 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 20 | 1.08 | 0.27 | 1.17 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 20 | 1.07 | 0.07 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 20 | 1.07 | 0.07 | 1.1 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 20 | 1.07 | 0.32 | 1.19 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 20 | 1.07 | 0.32 | 1.19 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 20 | 1.07 | 0.32 | 1.19 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 20 | 1.06 | 0.08 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 20 | 1.06 | 0.08 | 1.07 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 20 | 1.06 | 0.08 | 1.07 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 20 | 1.05 | 0.27 | 1.16 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 20 | 1.02 | 0.5 | 1.38 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 20 | 1.02 | 0.34 | 1.03 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 20 | 1.01 | 0.27 | 1.02 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 20 | 1.01 | 0.29 | 1.12 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 20 | 1.01 | 0.09 | 0.99 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 20 | 1.0 | 0.08 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 20 | 1.0 | 0.08 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 20 | 1.0 | 0.08 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 20 | 1.0 | 0.08 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 20 | 1.0 | 0.08 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 20 | 1.0 | 0.08 | 1.04 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 20 | 1.0 | 0.4 | 1.06 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 20 | 1.0 | 0.4 | 1.06 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 20 | 1.0 | 0.14 | 1.04 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 20 | 0.98 | 0.11 | 0.99 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 20 | 0.95 | 0.18 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 20 | 0.95 | 0.18 | 0.9 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 20 | 0.95 | 0.26 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 20 | 0.95 | 0.26 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 20 | 0.95 | 0.26 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 20 | 0.95 | 0.26 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 20 | 0.95 | 0.26 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 20 | 0.95 | 0.26 | 0.91 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 20 | 0.94 | 0.06 | 0.94 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 20 | 0.93 | 0.26 | 1.02 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 20 | 0.92 | 0.14 | 0.9 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 20 | 0.92 | 0.14 | 0.9 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 20 | 0.92 | 0.14 | 0.9 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 20 | 0.91 | 0.14 | 0.9 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 20 | 0.9 | 0.4 | 0.84 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 20 | 0.89 | 0.34 | 0.9 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 20 | 0.89 | 0.34 | 0.9 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 20 | 0.87 | 0.42 | 0.8 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 20 | 0.87 | 0.42 | 0.8 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 20 | 0.86 | 0.13 | 0.9 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 20 | 0.86 | 0.13 | 0.9 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 20 | 0.86 | 0.25 | 0.86 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 20 | 0.86 | 0.25 | 0.86 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 20 | 0.86 | 0.25 | 0.86 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 20 | 0.85 | 0.2 | 0.84 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 20 | 0.85 | 0.2 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 20 | 0.85 | 0.2 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 20 | 0.85 | 0.2 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 20 | 0.85 | 0.2 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 20 | 0.85 | 0.2 | 0.84 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 20 | 0.85 | 0.11 | 0.84 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 20 | 0.85 | 0.11 | 0.84 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 20 | 0.85 | 0.11 | 0.84 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 20 | 0.84 | 0.14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 20 | 0.84 | 0.14 | 0.89 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 20 | 0.84 | 0.06 | 0.83 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 20 | 0.83 | 0.31 | 0.82 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 20 | 0.83 | 0.31 | 0.82 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 20 | 0.82 | 0.09 | 0.82 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 20 | 0.82 | 0.09 | 0.82 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 20 | 0.82 | 0.09 | 0.82 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 20 | 0.81 | 0.21 | 0.84 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 20 | 0.81 | 0.1 | 0.82 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 20 | 0.8 | 0.21 | 0.81 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 20 | 0.8 | 0.21 | 0.81 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 20 | 0.8 | 0.21 | 0.81 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 20 | 0.8 | 0.3 | 0.76 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 20 | 0.8 | 0.07 | 0.8 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 20 | 0.8 | 0.07 | 0.8 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 20 | 0.8 | 0.07 | 0.8 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 20 | 0.78 | 0.33 | 0.67 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 20 | 0.78 | 0.33 | 0.67 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 20 | 0.78 | 0.33 | 0.67 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 20 | 0.78 | 0.32 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 20 | 0.78 | 0.32 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 20 | 0.78 | 0.32 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 20 | 0.78 | 0.2 | 0.8 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 20 | 0.78 | 0.2 | 0.8 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 20 | 0.78 | 0.2 | 0.8 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 20 | 0.77 | 0.06 | 0.77 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 20 | 0.77 | 0.09 | 0.78 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 20 | 0.75 | 0.35 | 0.97 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 20 | 0.75 | 0.15 | 0.72 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 20 | 0.74 | 0.5 | 0.46 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 20 | 0.73 | 0.1 | 0.73 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 20 | 0.72 | 0.31 | 0.78 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 20 | 0.72 | 0.31 | 0.78 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 20 | 0.72 | 0.16 | 0.65 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 20 | 0.72 | 0.16 | 0.65 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 20 | 0.72 | 0.16 | 0.65 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 20 | 0.71 | 0.21 | 0.61 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 20 | 0.71 | 0.21 | 0.61 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 20 | 0.71 | 0.21 | 0.61 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 20 | 0.7 | 0.62 | 0.44 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 20 | 0.7 | 0.16 | 0.68 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 20 | 0.7 | 0.06 | 0.71 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 20 | 0.69 | 0.26 | 0.7 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 20 | 0.69 | 0.26 | 0.7 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 20 | 0.69 | 0.26 | 0.7 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 20 | 0.69 | 0.33 | 0.7 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 20 | 0.69 | 0.11 | 0.66 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 20 | 0.69 | 0.11 | 0.66 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 20 | 0.69 | 0.11 | 0.66 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 20 | 0.68 | 0.29 | 0.67 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 20 | 0.68 | 0.14 | 0.66 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 20 | 0.67 | 0.16 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 20 | 0.67 | 0.16 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 20 | 0.67 | 0.16 | 0.72 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 20 | 0.66 | 0.17 | 0.62 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 20 | 0.66 | 0.26 | 0.66 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 20 | 0.66 | 0.26 | 0.66 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 20 | 0.65 | 0.11 | 0.64 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 20 | 0.65 | 0.11 | 0.64 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 20 | 0.65 | 0.21 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 20 | 0.65 | 0.21 | 0.67 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 20 | 0.65 | 0.21 | 0.64 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 20 | 0.65 | 0.21 | 0.64 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 20 | 0.65 | 0.11 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 20 | 0.65 | 0.11 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 20 | 0.65 | 0.11 | 0.65 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 20 | 0.65 | 0.21 | 0.66 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 20 | 0.65 | 0.21 | 0.66 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 20 | 0.65 | 0.21 | 0.66 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 20 | 0.65 | 0.21 | 0.66 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 20 | 0.65 | 0.21 | 0.66 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 20 | 0.65 | 0.21 | 0.66 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 20 | 0.64 | 0.12 | 0.66 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 20 | 0.64 | 0.12 | 0.66 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 20 | 0.64 | 0.12 | 0.66 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 20 | 0.63 | 0.15 | 0.66 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 20 | 0.62 | 0.18 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 20 | 0.62 | 0.2 | 0.64 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 20 | 0.62 | 0.2 | 0.64 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 20 | 0.62 | 0.18 | 0.68 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 20 | 0.62 | 0.18 | 0.68 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 20 | 0.62 | 0.18 | 0.68 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 20 | 0.62 | 0.18 | 0.68 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 20 | 0.62 | 0.18 | 0.68 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 20 | 0.62 | 0.18 | 0.68 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 20 | 0.62 | 0.04 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 20 | 0.62 | 0.04 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 20 | 0.62 | 0.04 | 0.62 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 20 | 0.61 | 0.15 | 0.6 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 20 | 0.61 | 0.15 | 0.6 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 20 | 0.6 | 0.25 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 20 | 0.59 | 0.08 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 20 | 0.59 | 0.08 | 0.62 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 20 | 0.59 | 0.28 | 0.5 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 20 | 0.57 | 0.23 | 0.49 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 20 | 0.57 | 0.05 | 0.56 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 20 | 0.56 | 0.05 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 20 | 0.56 | 0.05 | 0.58 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 20 | 0.56 | 0.12 | 0.55 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 20 | 0.56 | 0.23 | 0.53 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 20 | 0.55 | 0.08 | 0.55 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 20 | 0.55 | 0.1 | 0.52 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 20 | 0.55 | 0.1 | 0.52 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 20 | 0.55 | 0.1 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 20 | 0.54 | 0.05 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 20 | 0.54 | 0.05 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 20 | 0.54 | 0.05 | 0.54 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 20 | 0.54 | 0.1 | 0.55 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 20 | 0.53 | 0.16 | 0.57 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 20 | 0.53 | 0.16 | 0.57 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 20 | 0.53 | 0.16 | 0.57 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 20 | 0.53 | 0.05 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 20 | 0.53 | 0.05 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 20 | 0.53 | 0.05 | 0.52 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 20 | 0.53 | 0.06 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 20 | 0.53 | 0.06 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 20 | 0.53 | 0.06 | 0.5 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 20 | 0.53 | 0.21 | 0.52 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 20 | 0.52 | 0.21 | 0.44 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 20 | 0.52 | 0.21 | 0.44 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 20 | 0.52 | 0.21 | 0.44 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 20 | 0.52 | 0.21 | 0.44 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 20 | 0.52 | 0.21 | 0.44 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 20 | 0.52 | 0.21 | 0.44 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 20 | 0.52 | 0.19 | 0.52 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 20 | 0.52 | 0.19 | 0.52 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 20 | 0.52 | 0.19 | 0.52 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 20 | 0.52 | 0.35 | 0.39 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 20 | 0.51 | 0.19 | 0.53 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 20 | 0.5 | 0.15 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 20 | 0.5 | 0.1 | 0.53 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 20 | 0.5 | 0.1 | 0.53 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 20 | 0.5 | 0.1 | 0.53 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 20 | 0.5 | 0.1 | 0.53 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 20 | 0.5 | 0.1 | 0.53 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 20 | 0.5 | 0.1 | 0.53 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 20 | 0.5 | 0.14 | 0.51 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 20 | 0.49 | 0.11 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 20 | 0.49 | 0.11 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 20 | 0.49 | 0.11 | 0.44 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 20 | 0.49 | 0.22 | 0.44 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 20 | 0.49 | 0.09 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 20 | 0.49 | 0.09 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 20 | 0.49 | 0.09 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 20 | 0.49 | 0.09 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 20 | 0.49 | 0.09 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 20 | 0.49 | 0.09 | 0.52 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 20 | 0.49 | 0.07 | 0.5 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 20 | 0.49 | 0.19 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 20 | 0.49 | 0.19 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 20 | 0.49 | 0.19 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 20 | 0.49 | 0.14 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 20 | 0.49 | 0.14 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 20 | 0.49 | 0.14 | 0.44 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 20 | 0.49 | 0.13 | 0.47 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 20 | 0.49 | 0.13 | 0.47 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 20 | 0.47 | 0.11 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 20 | 0.47 | 0.11 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 20 | 0.47 | 0.11 | 0.52 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 20 | 0.47 | 0.11 | 0.45 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 20 | 0.47 | 0.11 | 0.45 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 20 | 0.47 | 0.11 | 0.45 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 20 | 0.46 | 0.06 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 20 | 0.46 | 0.06 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 20 | 0.46 | 0.06 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 20 | 0.46 | 0.09 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 20 | 0.46 | 0.09 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 20 | 0.46 | 0.09 | 0.45 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 20 | 0.46 | 0.18 | 0.43 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 20 | 0.46 | 0.18 | 0.43 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 20 | 0.46 | 0.18 | 0.43 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 20 | 0.45 | 0.11 | 0.46 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 20 | 0.45 | 0.11 | 0.46 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 20 | 0.45 | 0.08 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 20 | 0.44 | 0.13 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 20 | 0.44 | 0.13 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 20 | 0.44 | 0.13 | 0.44 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 20 | 0.44 | 0.1 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 20 | 0.44 | 0.1 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 20 | 0.44 | 0.1 | 0.45 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 20 | 0.44 | 0.21 | 0.4 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 20 | 0.43 | 0.07 | 0.46 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 20 | 0.43 | 0.13 | 0.42 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 20 | 0.43 | 0.13 | 0.42 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 20 | 0.43 | 0.18 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 20 | 0.43 | 0.18 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 20 | 0.43 | 0.18 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 20 | 0.42 | 0.04 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 20 | 0.42 | 0.04 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 20 | 0.42 | 0.04 | 0.44 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 20 | 0.42 | 0.08 | 0.44 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 20 | 0.41 | 0.17 | 0.38 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 20 | 0.39 | 0.1 | 0.38 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 20 | 0.39 | 0.13 | 0.4 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 20 | 0.39 | 0.13 | 0.34 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 20 | 0.39 | 0.1 | 0.35 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 20 | 0.38 | 0.09 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 20 | 0.37 | 0.08 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 20 | 0.37 | 0.08 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 20 | 0.37 | 0.08 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 20 | 0.37 | 0.05 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 20 | 0.37 | 0.05 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 20 | 0.37 | 0.05 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 20 | 0.37 | 0.05 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 20 | 0.37 | 0.05 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 20 | 0.37 | 0.05 | 0.38 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 20 | 0.35 | 0.1 | 0.38 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 20 | 0.35 | 0.12 | 0.34 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 20 | 0.35 | 0.12 | 0.32 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 20 | 0.35 | 0.12 | 0.32 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 20 | 0.35 | 0.12 | 0.32 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 20 | 0.34 | 0.13 | 0.34 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 20 | 0.34 | 0.13 | 0.34 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 20 | 0.34 | 0.13 | 0.34 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 20 | 0.33 | 0.16 | 0.29 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 20 | 0.33 | 0.16 | 0.29 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 20 | 0.33 | 0.17 | 0.33 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 20 | 0.33 | 0.17 | 0.33 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 20 | 0.33 | 0.04 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 20 | 0.33 | 0.04 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 20 | 0.33 | 0.04 | 0.34 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 20 | 0.33 | 0.03 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 20 | 0.33 | 0.03 | 0.32 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 20 | 0.31 | 0.06 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 20 | 0.31 | 0.06 | 0.3 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 20 | 0.3 | 0.17 | 0.28 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 20 | 0.29 | 0.03 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 20 | 0.29 | 0.03 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 20 | 0.29 | 0.03 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 20 | 0.29 | 0.09 | 0.26 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 20 | 0.28 | 0.09 | 0.29 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 20 | 0.28 | 0.09 | 0.29 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 20 | 0.28 | 0.09 | 0.29 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 20 | 0.28 | 0.04 | 0.28 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 20 | 0.28 | 0.08 | 0.29 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 20 | 0.28 | 0.08 | 0.29 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 20 | 0.28 | 0.08 | 0.29 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 20 | 0.28 | 0.09 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 20 | 0.28 | 0.07 | 0.26 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 20 | 0.27 | 0.02 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 20 | 0.27 | 0.02 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 20 | 0.27 | 0.02 | 0.28 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 20 | 0.27 | 0.05 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 20 | 0.27 | 0.05 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 20 | 0.27 | 0.05 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 20 | 0.27 | 0.05 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 20 | 0.27 | 0.05 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 20 | 0.27 | 0.05 | 0.26 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 20 | 0.26 | 0.05 | 0.28 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 20 | 0.26 | 0.12 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 20 | 0.25 | 0.06 | 0.26 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 20 | 0.25 | 0.06 | 0.26 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 20 | 0.25 | 0.06 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 20 | 0.25 | 0.04 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 20 | 0.25 | 0.04 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 20 | 0.25 | 0.04 | 0.26 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 20 | 0.25 | 0.05 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 20 | 0.25 | 0.05 | 0.22 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 20 | 0.24 | 0.03 | 0.25 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 20 | 0.24 | 0.06 | 0.23 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 20 | 0.24 | 0.09 | 0.24 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 20 | 0.24 | 0.09 | 0.24 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 20 | 0.23 | 0.06 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 20 | 0.23 | 0.06 | 0.23 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 20 | 0.23 | 0.06 | 0.23 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 20 | 0.23 | 0.06 | 0.24 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 20 | 0.23 | 0.06 | 0.24 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 20 | 0.23 | 0.03 | 0.23 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 20 | 0.23 | 0.02 | 0.22 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 20 | 0.23 | 0.04 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 20 | 0.22 | 0.05 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 20 | 0.22 | 0.05 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 20 | 0.22 | 0.05 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 20 | 0.22 | 0.05 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 20 | 0.22 | 0.05 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 20 | 0.22 | 0.05 | 0.22 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 20 | 0.22 | 0.03 | 0.22 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 20 | 0.21 | 0.01 | 0.21 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 20 | 0.2 | 0.04 | 0.2 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 20 | 0.2 | 0.04 | 0.2 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 20 | 0.2 | 0.03 | 0.21 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 20 | 0.18 | 0.02 | 0.19 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 20 | 0.17 | 0.05 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 20 | 0.16 | 0.03 | 0.16 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 20 | 0.16 | 0.03 | 0.16 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 20 | 0.15 | 0.05 | 0.14 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 20 | 0.15 | 0.05 | 0.14 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 20 | 0.11 | 0.01 | 0.11 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 19 | 1.31 | 0.62 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 19 | 1.31 | 0.62 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 19 | 1.31 | 0.62 | 1.32 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 19 | 1.28 | 0.58 | 1.19 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 19 | 1.28 | 0.58 | 1.19 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 19 | 1.13 | 0.34 | 1.09 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 19 | 1.13 | 0.34 | 1.09 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 19 | 1.13 | 0.34 | 1.09 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 19 | 1.13 | 0.34 | 1.09 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 19 | 1.13 | 0.34 | 1.09 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 19 | 1.13 | 0.34 | 1.09 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 19 | 1.04 | 0.41 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 19 | 1.04 | 0.41 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 19 | 1.04 | 0.41 | 1.11 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 19 | 0.97 | 0.62 | 0.89 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 19 | 0.96 | 0.12 | 0.96 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 19 | 0.96 | 0.12 | 0.96 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 19 | 0.96 | 0.23 | 1.04 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 19 | 0.92 | 0.34 | 0.95 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 19 | 0.92 | 0.34 | 0.95 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 19 | 0.92 | 0.34 | 0.95 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 19 | 0.9 | 0.39 | 0.79 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 19 | 0.86 | 0.17 | 0.87 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 19 | 0.86 | 0.17 | 0.87 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 19 | 0.86 | 0.17 | 0.87 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 19 | 0.85 | 0.25 | 0.88 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 19 | 0.85 | 0.25 | 0.88 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 19 | 0.85 | 0.25 | 0.88 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 19 | 0.85 | 0.25 | 0.88 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 19 | 0.85 | 0.25 | 0.88 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 19 | 0.85 | 0.25 | 0.88 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 19 | 0.84 | 0.23 | 0.75 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 19 | 0.84 | 0.17 | 0.9 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 19 | 0.77 | 0.43 | 0.59 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 19 | 0.77 | 0.43 | 0.59 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 19 | 0.77 | 0.43 | 0.59 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 19 | 0.71 | 0.14 | 0.73 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 19 | 0.71 | 0.14 | 0.73 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 19 | 0.71 | 0.14 | 0.73 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 19 | 0.68 | 0.47 | 0.94 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 19 | 0.68 | 0.47 | 0.94 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 19 | 0.67 | 0.15 | 0.67 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 19 | 0.67 | 0.15 | 0.67 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 19 | 0.67 | 0.15 | 0.67 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 19 | 0.67 | 0.15 | 0.67 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 19 | 0.67 | 0.15 | 0.67 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 19 | 0.67 | 0.15 | 0.67 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 19 | 0.62 | 0.23 | 0.63 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 19 | 0.59 | 0.24 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 19 | 0.59 | 0.24 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 19 | 0.59 | 0.24 | 0.54 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 19 | 0.58 | 0.12 | 0.62 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 19 | 0.58 | 0.12 | 0.62 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 19 | 0.56 | 0.26 | 0.53 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 19 | 0.56 | 0.26 | 0.53 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 19 | 0.56 | 0.26 | 0.53 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 19 | 0.55 | 0.11 | 0.58 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 19 | 0.55 | 0.11 | 0.58 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 19 | 0.55 | 0.11 | 0.58 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 19 | 0.55 | 0.09 | 0.55 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 19 | 0.53 | 0.14 | 0.55 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 19 | 0.52 | 0.17 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 19 | 0.52 | 0.17 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 19 | 0.52 | 0.17 | 0.54 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 19 | 0.52 | 0.23 | 0.49 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 19 | 0.52 | 0.23 | 0.49 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 19 | 0.52 | 0.23 | 0.49 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 19 | 0.51 | 0.12 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 19 | 0.51 | 0.12 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 19 | 0.51 | 0.12 | 0.53 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 19 | 0.48 | 0.15 | 0.47 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 19 | 0.47 | 0.22 | 0.41 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 19 | 0.47 | 0.22 | 0.41 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 19 | 0.47 | 0.22 | 0.41 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 19 | 0.47 | 0.22 | 0.41 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 19 | 0.47 | 0.22 | 0.41 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 19 | 0.47 | 0.22 | 0.41 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 19 | 0.43 | 0.1 | 0.45 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 19 | 0.4 | 0.25 | 0.35 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 19 | 0.4 | 0.25 | 0.35 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 19 | 0.4 | 0.25 | 0.35 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 19 | 0.39 | 0.13 | 0.41 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 19 | 0.39 | 0.13 | 0.41 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 19 | 0.39 | 0.13 | 0.41 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 19 | 0.37 | 0.19 | 0.32 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 19 | 0.37 | 0.19 | 0.32 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 19 | 0.37 | 0.19 | 0.32 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 19 | 0.35 | 0.13 | 0.41 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 19 | 0.34 | 0.14 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 19 | 0.34 | 0.14 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 19 | 0.34 | 0.14 | 0.31 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 19 | 0.34 | 0.11 | 0.35 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 19 | 0.32 | 0.17 | 0.29 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 19 | 0.32 | 0.17 | 0.29 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 19 | 0.31 | 0.18 | 0.22 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 19 | 0.31 | 0.13 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 19 | 0.29 | 0.09 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 19 | 0.29 | 0.09 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 19 | 0.29 | 0.09 | 0.28 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 19 | 0.28 | 0.06 | 0.27 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 19 | 0.27 | 0.05 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 19 | 0.25 | 0.05 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 19 | 0.25 | 0.05 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 19 | 0.25 | 0.05 | 0.25 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 19 | 0.22 | 0.07 | 0.23 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 19 | 0.22 | 0.05 | 0.23 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 19 | 0.22 | 0.05 | 0.23 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 19 | 0.22 | 0.05 | 0.23 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 19 | 0.2 | 0.05 | 0.18 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 19 | 0.2 | 0.06 | 0.19 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 19 | 0.2 | 0.06 | 0.19 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 19 | 0.2 | 0.06 | 0.19 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 19 | 0.18 | 0.06 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 19 | 0.18 | 0.06 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 19 | 0.18 | 0.06 | 0.16 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 18 | 1.56 | 1.03 | 1.27 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 18 | 1.56 | 1.03 | 1.27 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 18 | 1.15 | 0.58 | 1.02 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 18 | 1.15 | 0.58 | 1.02 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 18 | 1.13 | 0.51 | 1.36 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 18 | 1.13 | 0.51 | 1.36 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 18 | 1.13 | 0.51 | 1.36 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 18 | 1.13 | 0.51 | 1.36 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 18 | 1.13 | 0.51 | 1.36 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 18 | 1.13 | 0.51 | 1.36 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 18 | 1.07 | 0.23 | 1.15 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 18 | 1.05 | 0.6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 18 | 1.05 | 0.6 | 1.06 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 18 | 0.97 | 0.31 | 0.96 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 18 | 0.97 | 0.31 | 0.96 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 18 | 0.69 | 0.08 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 18 | 0.69 | 0.08 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 18 | 0.69 | 0.08 | 0.7 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 18 | 0.69 | 0.08 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 18 | 0.69 | 0.08 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 18 | 0.69 | 0.08 | 0.7 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 18 | 0.68 | 0.42 | 0.49 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 18 | 0.68 | 0.42 | 0.49 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 18 | 0.68 | 0.42 | 0.49 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 18 | 0.68 | 0.42 | 0.49 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 18 | 0.68 | 0.42 | 0.49 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 18 | 0.68 | 0.42 | 0.49 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 18 | 0.59 | 0.34 | 0.59 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 18 | 0.59 | 0.34 | 0.59 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 18 | 0.59 | 0.34 | 0.59 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 18 | 0.51 | 0.22 | 0.5 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 18 | 0.51 | 0.16 | 0.49 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 18 | 0.49 | 0.21 | 0.49 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 18 | 0.49 | 0.21 | 0.49 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 18 | 0.49 | 0.21 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 18 | 0.47 | 0.06 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 18 | 0.47 | 0.06 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 18 | 0.47 | 0.06 | 0.48 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 18 | 0.46 | 0.19 | 0.42 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 18 | 0.46 | 0.19 | 0.42 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 18 | 0.44 | 0.1 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 18 | 0.44 | 0.1 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 18 | 0.44 | 0.1 | 0.46 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 18 | 0.42 | 0.1 | 0.4 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 18 | 0.4 | 0.14 | 0.38 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 18 | 0.4 | 0.14 | 0.38 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 18 | 0.4 | 0.14 | 0.38 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 18 | 0.32 | 0.14 | 0.29 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 18 | 0.32 | 0.14 | 0.29 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 18 | 0.32 | 0.14 | 0.29 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 18 | 0.32 | 0.09 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 18 | 0.32 | 0.09 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 18 | 0.32 | 0.09 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 18 | 0.32 | 0.09 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 18 | 0.29 | 0.06 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 18 | 0.29 | 0.06 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 18 | 0.29 | 0.06 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 18 | 0.29 | 0.06 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 18 | 0.29 | 0.06 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 18 | 0.29 | 0.06 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 18 | 0.28 | 0.08 | 0.3 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 18 | 0.28 | 0.08 | 0.3 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 18 | 0.28 | 0.08 | 0.3 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 18 | 0.24 | 0.05 | 0.24 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 18 | 0.2 | 0.06 | 0.2 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 18 | 0.2 | 0.06 | 0.2 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 18 | 0.2 | 0.06 | 0.2 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 18 | 0.19 | 0.04 | 0.19 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 18 | 0.19 | 0.04 | 0.19 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 17 | 2.24 | 0.72 | 1.99 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 17 | 2.24 | 0.72 | 1.99 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 17 | 1.31 | 0.03 | 1.31 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 17 | 1.17 | 0.03 | 1.18 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 17 | 0.93 | 0.09 | 0.92 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 17 | 0.93 | 0.09 | 0.92 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 17 | 0.93 | 0.09 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 17 | 0.88 | 0.04 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 17 | 0.88 | 0.04 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 17 | 0.88 | 0.04 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 17 | 0.88 | 0.04 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 17 | 0.88 | 0.04 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 17 | 0.88 | 0.04 | 0.88 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 17 | 0.84 | 0.29 | 0.76 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 17 | 0.79 | 0.43 | 0.79 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 17 | 0.74 | 0.03 | 0.74 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 17 | 0.61 | 0.29 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 17 | 0.59 | 0.24 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 17 | 0.59 | 0.24 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 17 | 0.59 | 0.24 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 17 | 0.59 | 0.24 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 17 | 0.59 | 0.24 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 17 | 0.59 | 0.24 | 0.58 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 17 | 0.5 | 0.12 | 0.53 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 17 | 0.45 | 0.28 | 0.36 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 17 | 0.45 | 0.02 | 0.44 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 17 | 0.43 | 0.2 | 0.41 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 17 | 0.38 | 0.08 | 0.39 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 17 | 0.36 | 0.13 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 17 | 0.36 | 0.13 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 17 | 0.36 | 0.13 | 0.36 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 17 | 0.34 | 0.13 | 0.35 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 17 | 0.33 | 0.12 | 0.35 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 17 | 0.33 | 0.12 | 0.35 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 17 | 0.31 | 0.07 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 17 | 0.31 | 0.07 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 17 | 0.31 | 0.07 | 0.33 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 17 | 0.31 | 0.08 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 17 | 0.31 | 0.08 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 17 | 0.31 | 0.08 | 0.31 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 17 | 0.3 | 0.08 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 17 | 0.29 | 0.07 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 17 | 0.29 | 0.07 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 17 | 0.29 | 0.07 | 0.29 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 17 | 0.28 | 0.1 | 0.27 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 17 | 0.28 | 0.1 | 0.27 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 17 | 0.28 | 0.1 | 0.27 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 17 | 0.28 | 0.01 | 0.28 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 17 | 0.27 | 0.06 | 0.26 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 17 | 0.26 | 0.07 | 0.24 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 17 | 0.26 | 0.1 | 0.28 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 17 | 0.26 | 0.1 | 0.28 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 17 | 0.26 | 0.1 | 0.28 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 17 | 0.22 | 0.08 | 0.21 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 17 | 0.21 | 0.06 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 17 | 0.21 | 0.06 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 17 | 0.21 | 0.06 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 17 | 0.21 | 0.06 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 17 | 0.21 | 0.06 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 17 | 0.21 | 0.06 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 17 | 0.21 | 0.06 | 0.22 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 17 | 0.2 | 0.04 | 0.21 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 17 | 0.19 | 0.06 | 0.17 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 17 | 0.18 | 0.07 | 0.16 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 17 | 0.16 | 0.05 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 17 | 0.16 | 0.05 | 0.13 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 17 | 0.12 | 0.02 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 17 | 0.12 | 0.02 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 17 | 0.12 | 0.02 | 0.11 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 16 | 1.15 | 0.34 | 1.15 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 16 | 0.94 | 0.62 | 0.9 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 16 | 0.65 | 0.33 | 0.82 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 16 | 0.64 | 0.15 | 0.62 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 16 | 0.58 | 0.29 | 0.56 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 16 | 0.55 | 0.38 | 0.45 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 16 | 0.49 | 0.23 | 0.48 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 16 | 0.45 | 0.18 | 0.44 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 16 | 0.43 | 0.25 | 0.38 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 16 | 0.43 | 0.25 | 0.38 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 16 | 0.43 | 0.25 | 0.38 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 16 | 0.42 | 0.19 | 0.39 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 16 | 0.42 | 0.19 | 0.39 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 16 | 0.35 | 0.17 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 16 | 0.35 | 0.17 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 16 | 0.35 | 0.17 | 0.29 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 16 | 0.35 | 0.19 | 0.28 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 16 | 0.35 | 0.19 | 0.28 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 16 | 0.35 | 0.19 | 0.28 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 16 | 0.3 | 0.1 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 16 | 0.3 | 0.1 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 16 | 0.3 | 0.1 | 0.3 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 16 | 0.3 | 0.11 | 0.29 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 16 | 0.3 | 0.11 | 0.29 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 16 | 0.3 | 0.11 | 0.29 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 16 | 0.3 | 0.11 | 0.29 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 16 | 0.3 | 0.11 | 0.29 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 16 | 0.3 | 0.11 | 0.29 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 16 | 0.29 | 0.05 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 16 | 0.29 | 0.05 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 16 | 0.29 | 0.05 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 16 | 0.29 | 0.05 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 16 | 0.29 | 0.05 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 16 | 0.29 | 0.05 | 0.28 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 16 | 0.25 | 0.16 | 0.2 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 16 | 0.25 | 0.16 | 0.2 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 16 | 0.25 | 0.16 | 0.2 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 16 | 0.24 | 0.08 | 0.22 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 16 | 0.24 | 0.08 | 0.22 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 16 | 0.24 | 0.08 | 0.22 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 16 | 0.24 | 0.09 | 0.28 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 16 | 0.23 | 0.16 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 16 | 0.21 | 0.05 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 16 | 0.21 | 0.05 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 16 | 0.21 | 0.05 | 0.2 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 16 | 0.21 | 0.06 | 0.22 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 16 | 0.19 | 0.07 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 16 | 0.19 | 0.07 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 16 | 0.19 | 0.07 | 0.16 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 16 | 0.15 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 15 | 1.44 | 0.95 | 1.26 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 15 | 1.44 | 0.95 | 1.26 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 15 | 1.2 | 0.85 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 15 | 1.2 | 0.85 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 15 | 1.2 | 0.85 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 15 | 1.2 | 0.85 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 15 | 1.2 | 0.85 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 15 | 1.2 | 0.85 | 1.17 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 15 | 1.1 | 0.4 | 1.22 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 15 | 1.1 | 0.4 | 1.22 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 15 | 1.1 | 0.45 | 1.03 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 15 | 1.09 | 0.47 | 1.06 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 15 | 1.09 | 0.47 | 1.06 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 15 | 1.01 | 0.3 | 0.95 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 15 | 0.8 | 0.45 | 0.68 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 15 | 0.75 | 0.24 | 0.85 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 15 | 0.74 | 0.47 | 0.59 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 15 | 0.74 | 0.47 | 0.59 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 15 | 0.74 | 0.47 | 0.59 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 15 | 0.72 | 0.28 | 0.85 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 15 | 0.69 | 0.38 | 0.6 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 15 | 0.69 | 0.38 | 0.6 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 15 | 0.64 | 0.58 | 0.58 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 15 | 0.64 | 0.58 | 0.58 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 15 | 0.53 | 0.31 | 0.56 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 15 | 0.53 | 0.36 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 15 | 0.53 | 0.36 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 15 | 0.53 | 0.36 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 15 | 0.53 | 0.36 | 0.36 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 15 | 0.49 | 0.28 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 15 | 0.48 | 0.19 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 15 | 0.48 | 0.19 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 15 | 0.48 | 0.19 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 15 | 0.48 | 0.19 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 15 | 0.48 | 0.19 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 15 | 0.48 | 0.19 | 0.52 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 15 | 0.45 | 0.14 | 0.5 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 15 | 0.45 | 0.08 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 15 | 0.45 | 0.08 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 15 | 0.45 | 0.08 | 0.42 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 15 | 0.4 | 0.16 | 0.35 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 15 | 0.4 | 0.18 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 15 | 0.4 | 0.18 | 0.41 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 15 | 0.39 | 0.21 | 0.36 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 15 | 0.39 | 0.21 | 0.36 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 15 | 0.39 | 0.21 | 0.36 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 15 | 0.36 | 0.1 | 0.33 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 15 | 0.36 | 0.1 | 0.33 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 15 | 0.36 | 0.1 | 0.33 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 15 | 0.36 | 0.01 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 15 | 0.36 | 0.01 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 15 | 0.36 | 0.01 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 15 | 0.34 | 0.12 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 15 | 0.34 | 0.12 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 15 | 0.34 | 0.12 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 15 | 0.34 | 0.12 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 15 | 0.34 | 0.12 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 15 | 0.34 | 0.12 | 0.31 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 15 | 0.31 | 0.13 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 15 | 0.31 | 0.13 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 15 | 0.31 | 0.13 | 0.32 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 15 | 0.3 | 0.18 | 0.23 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 15 | 0.29 | 0.11 | 0.29 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 15 | 0.29 | 0.11 | 0.29 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 15 | 0.29 | 0.11 | 0.29 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 15 | 0.29 | 0.11 | 0.26 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 15 | 0.29 | 0.11 | 0.28 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 15 | 0.23 | 0.09 | 0.21 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 15 | 0.23 | 0.09 | 0.21 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 15 | 0.23 | 0.09 | 0.21 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 15 | 0.19 | 0.07 | 0.18 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 15 | 0.18 | 0.05 | 0.18 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 15 | 0.15 | 0.03 | 0.14 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 15 | 0.14 | 0.04 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 15 | 0.14 | 0.04 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 15 | 0.14 | 0.04 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 15 | 0.13 | 0.02 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 15 | 0.13 | 0.02 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 15 | 0.13 | 0.01 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 15 | 0.13 | 0.01 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 15 | 0.13 | 0.01 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 15 | 0.13 | 0.01 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 15 | 0.13 | 0.01 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 15 | 0.13 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 14 | 1.21 | 0.46 | 1.35 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 14 | 1.01 | 0.56 | 1.14 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 14 | 1.01 | 0.56 | 1.14 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 14 | 0.68 | 0.13 | 0.74 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 14 | 0.63 | 0.35 | 0.64 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 14 | 0.63 | 0.35 | 0.64 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 14 | 0.63 | 0.35 | 0.64 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 14 | 0.62 | 0.48 | 0.43 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 14 | 0.62 | 0.48 | 0.43 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 14 | 0.53 | 0.22 | 0.6 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 14 | 0.53 | 0.22 | 0.6 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 14 | 0.52 | 0.42 | 0.4 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 14 | 0.52 | 0.42 | 0.4 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 14 | 0.47 | 0.24 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 14 | 0.47 | 0.24 | 0.38 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 14 | 0.46 | 0.08 | 0.48 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 14 | 0.46 | 0.18 | 0.5 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 14 | 0.4 | 0.26 | 0.31 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 14 | 0.4 | 0.26 | 0.31 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 14 | 0.4 | 0.26 | 0.31 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 14 | 0.38 | 0.17 | 0.37 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 14 | 0.37 | 0.15 | 0.36 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 14 | 0.37 | 0.15 | 0.36 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 14 | 0.29 | 0.08 | 0.29 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 14 | 0.25 | 0.1 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 14 | 0.25 | 0.1 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 14 | 0.25 | 0.1 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 14 | 0.25 | 0.1 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 14 | 0.25 | 0.1 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 14 | 0.25 | 0.1 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 14 | 0.23 | 0.07 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 14 | 0.23 | 0.07 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 14 | 0.23 | 0.07 | 0.22 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 14 | 0.21 | 0.17 | 0.17 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 14 | 0.21 | 0.17 | 0.17 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 14 | 0.2 | 0.05 | 0.19 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 14 | 0.19 | 0.06 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 14 | 0.19 | 0.06 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 14 | 0.19 | 0.06 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 14 | 0.19 | 0.06 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 14 | 0.19 | 0.06 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 14 | 0.19 | 0.06 | 0.17 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 14 | 0.19 | 0.01 | 0.19 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 14 | 0.18 | 0.05 | 0.18 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 14 | 0.18 | 0.03 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 14 | 0.18 | 0.03 | 0.2 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 14 | 0.15 | 0.03 | 0.16 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 14 | 0.15 | 0.05 | 0.14 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 13 | 1.49 | 0.79 | 1.51 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 13 | 1.49 | 0.79 | 1.51 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 13 | 1.11 | 0.55 | 1.16 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 13 | 1.11 | 0.55 | 1.16 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 13 | 1.11 | 0.55 | 1.16 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 13 | 1.11 | 0.55 | 1.16 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 13 | 1.11 | 0.55 | 1.16 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 13 | 1.11 | 0.55 | 1.16 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 13 | 0.98 | 0.41 | 1.0 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 13 | 0.75 | 0.21 | 0.8 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 13 | 0.74 | 0.36 | 0.62 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 13 | 0.74 | 0.36 | 0.62 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 13 | 0.74 | 0.36 | 0.62 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 13 | 0.74 | 0.36 | 0.62 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 13 | 0.74 | 0.36 | 0.62 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 13 | 0.74 | 0.36 | 0.62 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 13 | 0.62 | 0.32 | 0.62 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 13 | 0.62 | 0.32 | 0.62 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 13 | 0.62 | 0.32 | 0.62 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 13 | 0.58 | 0.23 | 0.62 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 13 | 0.58 | 0.23 | 0.62 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 13 | 0.58 | 0.23 | 0.62 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 13 | 0.56 | 0.56 | 0.44 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 13 | 0.42 | 0.17 | 0.43 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 13 | 0.42 | 0.17 | 0.43 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 13 | 0.42 | 0.17 | 0.43 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 13 | 0.39 | 0.18 | 0.35 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 13 | 0.38 | 0.14 | 0.38 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 13 | 0.37 | 0.1 | 0.35 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 13 | 0.37 | 0.1 | 0.35 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 13 | 0.37 | 0.1 | 0.35 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 13 | 0.3 | 0.1 | 0.34 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 13 | 0.3 | 0.1 | 0.34 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 13 | 0.25 | 0.17 | 0.2 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 13 | 0.25 | 0.17 | 0.2 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 13 | 0.25 | 0.17 | 0.2 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 13 | 0.24 | 0.1 | 0.21 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 13 | 0.24 | 0.05 | 0.23 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 13 | 0.22 | 0.07 | 0.2 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 13 | 0.2 | 0.07 | 0.19 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 13 | 0.2 | 0.07 | 0.19 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 13 | 0.2 | 0.07 | 0.19 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 13 | 0.18 | 0.07 | 0.15 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 13 | 0.17 | 0.04 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 13 | 0.17 | 0.04 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 13 | 0.17 | 0.04 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 13 | 0.17 | 0.04 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 13 | 0.17 | 0.04 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 13 | 0.17 | 0.04 | 0.17 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 13 | 0.15 | 0.03 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 13 | 0.15 | 0.03 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 13 | 0.15 | 0.03 | 0.15 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 13 | 0.14 | 0.03 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 13 | 0.14 | 0.02 | 0.14 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 13 | 0.14 | 0.02 | 0.14 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 13 | 0.12 | 0.02 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 13 | 0.12 | 0.02 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 12 | 1.12 | 0.65 | 1.15 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 12 | 1.12 | 0.65 | 1.15 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 12 | 1.05 | 0.66 | 0.82 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 12 | 1.05 | 0.66 | 0.82 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 12 | 1.05 | 0.66 | 0.82 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 12 | 0.71 | 0.49 | 0.57 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 12 | 0.71 | 0.49 | 0.57 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 12 | 0.71 | 0.43 | 0.7 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 12 | 0.68 | 0.3 | 0.56 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 12 | 0.68 | 0.3 | 0.56 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 12 | 0.68 | 0.3 | 0.56 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 12 | 0.68 | 0.3 | 0.56 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 12 | 0.66 | 0.47 | 0.42 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 12 | 0.66 | 0.47 | 0.42 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 12 | 0.64 | 0.26 | 0.67 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 12 | 0.63 | 0.33 | 0.8 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 12 | 0.58 | 0.32 | 0.52 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 12 | 0.58 | 0.32 | 0.52 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 12 | 0.51 | 0.34 | 0.38 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 12 | 0.5 | 0.22 | 0.52 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 12 | 0.5 | 0.22 | 0.52 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 12 | 0.5 | 0.22 | 0.52 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 12 | 0.5 | 0.22 | 0.52 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 12 | 0.48 | 0.22 | 0.48 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 12 | 0.48 | 0.22 | 0.48 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 12 | 0.48 | 0.22 | 0.48 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 12 | 0.48 | 0.22 | 0.48 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 12 | 0.48 | 0.22 | 0.48 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 12 | 0.48 | 0.22 | 0.48 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 12 | 0.44 | 0.33 | 0.3 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 12 | 0.44 | 0.33 | 0.3 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 12 | 0.42 | 0.21 | 0.44 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 12 | 0.42 | 0.21 | 0.44 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 12 | 0.42 | 0.21 | 0.44 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 12 | 0.4 | 0.17 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 12 | 0.4 | 0.17 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 12 | 0.4 | 0.17 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 12 | 0.4 | 0.17 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 12 | 0.4 | 0.17 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 12 | 0.4 | 0.17 | 0.4 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 12 | 0.38 | 0.14 | 0.38 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 12 | 0.38 | 0.14 | 0.38 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 12 | 0.38 | 0.14 | 0.38 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 12 | 0.34 | 0.1 | 0.36 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 12 | 0.34 | 0.1 | 0.36 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 12 | 0.34 | 0.1 | 0.36 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 12 | 0.34 | 0.16 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 12 | 0.34 | 0.16 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 12 | 0.34 | 0.16 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 12 | 0.34 | 0.16 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 12 | 0.34 | 0.16 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 12 | 0.34 | 0.16 | 0.34 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 12 | 0.34 | 0.11 | 0.32 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 12 | 0.34 | 0.11 | 0.32 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 12 | 0.34 | 0.11 | 0.32 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 12 | 0.32 | 0.17 | 0.26 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 12 | 0.32 | 0.13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 12 | 0.32 | 0.13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 12 | 0.32 | 0.13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 12 | 0.32 | 0.13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 12 | 0.32 | 0.13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 12 | 0.32 | 0.13 | 0.3 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 12 | 0.31 | 0.14 | 0.29 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 12 | 0.31 | 0.14 | 0.29 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 12 | 0.29 | 0.13 | 0.25 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 12 | 0.29 | 0.13 | 0.25 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 12 | 0.29 | 0.13 | 0.25 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 12 | 0.27 | 0.14 | 0.2 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 12 | 0.27 | 0.14 | 0.2 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 12 | 0.27 | 0.14 | 0.2 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 12 | 0.26 | 0.16 | 0.18 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 12 | 0.26 | 0.1 | 0.25 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 12 | 0.26 | 0.1 | 0.25 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 12 | 0.26 | 0.1 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 12 | 0.23 | 0.1 | 0.24 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 12 | 0.23 | 0.1 | 0.24 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 12 | 0.23 | 0.1 | 0.24 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 12 | 0.23 | 0.05 | 0.22 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 12 | 0.23 | 0.1 | 0.23 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 12 | 0.22 | 0.05 | 0.22 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 12 | 0.22 | 0.05 | 0.22 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 12 | 0.22 | 0.05 | 0.22 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 12 | 0.2 | 0.08 | 0.17 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 12 | 0.18 | 0.06 | 0.2 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 12 | 0.18 | 0.06 | 0.2 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 12 | 0.18 | 0.06 | 0.2 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 12 | 0.18 | 0.04 | 0.19 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 12 | 0.16 | 0.02 | 0.15 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 12 | 0.14 | 0.03 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 11 | 1.75 | 0.33 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 11 | 1.75 | 0.33 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 11 | 1.75 | 0.33 | 1.7 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 11 | 1.14 | 0.74 | 0.96 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 11 | 1.06 | 0.17 | 1.01 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 11 | 0.87 | 0.44 | 1.02 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 11 | 0.87 | 0.44 | 1.02 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 11 | 0.87 | 0.44 | 1.02 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 11 | 0.87 | 0.44 | 1.02 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 11 | 0.82 | 0.19 | 0.77 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 11 | 0.79 | 0.41 | 0.64 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 11 | 0.79 | 0.41 | 0.64 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 11 | 0.73 | 0.23 | 0.75 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 11 | 0.73 | 0.23 | 0.75 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 11 | 0.73 | 0.23 | 0.75 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 11 | 0.63 | 0.45 | 0.47 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 11 | 0.63 | 0.45 | 0.47 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 11 | 0.63 | 0.45 | 0.47 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 11 | 0.59 | 0.32 | 0.73 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 11 | 0.59 | 0.32 | 0.73 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 11 | 0.59 | 0.32 | 0.73 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 11 | 0.57 | 0.28 | 0.53 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 11 | 0.48 | 0.18 | 0.43 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 11 | 0.45 | 0.13 | 0.51 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 11 | 0.43 | 0.24 | 0.39 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 11 | 0.43 | 0.24 | 0.39 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 11 | 0.43 | 0.05 | 0.44 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 11 | 0.4 | 0.25 | 0.34 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 11 | 0.4 | 0.25 | 0.34 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 11 | 0.4 | 0.25 | 0.34 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 11 | 0.39 | 0.25 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 11 | 0.39 | 0.25 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 11 | 0.39 | 0.25 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 11 | 0.39 | 0.25 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 11 | 0.39 | 0.25 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 11 | 0.39 | 0.25 | 0.22 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 11 | 0.38 | 0.17 | 0.32 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 11 | 0.38 | 0.18 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 11 | 0.38 | 0.18 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 11 | 0.38 | 0.18 | 0.39 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 11 | 0.37 | 0.16 | 0.33 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 11 | 0.37 | 0.16 | 0.33 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 11 | 0.34 | 0.14 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 11 | 0.34 | 0.14 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 11 | 0.34 | 0.14 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 11 | 0.3 | 0.08 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 11 | 0.3 | 0.08 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 11 | 0.3 | 0.08 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 11 | 0.3 | 0.08 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 11 | 0.3 | 0.08 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 11 | 0.3 | 0.08 | 0.32 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 11 | 0.3 | 0.1 | 0.31 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 11 | 0.29 | 0.1 | 0.3 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 11 | 0.29 | 0.1 | 0.3 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 11 | 0.26 | 0.12 | 0.22 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 11 | 0.26 | 0.12 | 0.22 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 11 | 0.26 | 0.12 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 11 | 0.25 | 0.08 | 0.24 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 11 | 0.25 | 0.08 | 0.24 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 11 | 0.25 | 0.08 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 11 | 0.24 | 0.07 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 11 | 0.24 | 0.07 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 11 | 0.24 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 11 | 0.24 | 0.07 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 11 | 0.24 | 0.07 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 11 | 0.24 | 0.07 | 0.24 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 11 | 0.23 | 0.09 | 0.21 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 11 | 0.23 | 0.09 | 0.21 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 11 | 0.23 | 0.09 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 11 | 0.2 | 0.04 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 11 | 0.2 | 0.04 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 11 | 0.2 | 0.04 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 11 | 0.2 | 0.04 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 11 | 0.2 | 0.04 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 11 | 0.2 | 0.04 | 0.21 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 11 | 0.18 | 0.05 | 0.16 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 11 | 0.16 | 0.05 | 0.17 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 11 | 0.16 | 0.05 | 0.17 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 11 | 0.16 | 0.05 | 0.17 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 11 | 0.16 | 0.04 | 0.15 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 11 | 0.16 | 0.03 | 0.15 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 11 | 0.15 | 0.03 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 11 | 0.15 | 0.03 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 11 | 0.15 | 0.03 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 11 | 0.15 | 0.03 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 11 | 0.15 | 0.03 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 11 | 0.15 | 0.03 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 11 | 0.13 | 0.01 | 0.14 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 11 | 0.12 | 0.02 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 11 | 0.12 | 0.02 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 11 | 0.12 | 0.02 | 0.12 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 10 | 1.03 | 0.34 | 1.0 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 10 | 1.03 | 0.34 | 1.0 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 10 | 0.85 | 0.14 | 0.88 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 10 | 0.85 | 0.14 | 0.88 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 10 | 0.85 | 0.14 | 0.88 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 10 | 0.83 | 0.59 | 0.68 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 10 | 0.83 | 0.59 | 0.68 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 10 | 0.83 | 0.59 | 0.68 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 10 | 0.83 | 0.59 | 0.68 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 10 | 0.79 | 0.07 | 0.8 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 10 | 0.79 | 0.07 | 0.8 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 10 | 0.79 | 0.07 | 0.8 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 10 | 0.79 | 0.07 | 0.8 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 10 | 0.79 | 0.07 | 0.8 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 10 | 0.79 | 0.07 | 0.8 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 10 | 0.72 | 0.39 | 0.64 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 10 | 0.7 | 0.32 | 0.68 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 10 | 0.6 | 0.17 | 0.63 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 10 | 0.6 | 0.17 | 0.63 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 10 | 0.6 | 0.17 | 0.63 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 10 | 0.6 | 0.17 | 0.63 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 10 | 0.6 | 0.17 | 0.63 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 10 | 0.6 | 0.17 | 0.63 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 10 | 0.58 | 0.41 | 0.39 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 10 | 0.58 | 0.41 | 0.39 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 10 | 0.58 | 0.41 | 0.39 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 10 | 0.58 | 0.41 | 0.39 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 10 | 0.58 | 0.41 | 0.39 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 10 | 0.58 | 0.41 | 0.39 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 10 | 0.53 | 0.29 | 0.57 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 10 | 0.53 | 0.29 | 0.57 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 10 | 0.53 | 0.4 | 0.48 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 10 | 0.53 | 0.4 | 0.48 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 10 | 0.53 | 0.4 | 0.48 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 10 | 0.52 | 0.36 | 0.5 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 10 | 0.47 | 0.14 | 0.5 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 10 | 0.47 | 0.14 | 0.5 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 10 | 0.41 | 0.15 | 0.39 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 10 | 0.38 | 0.15 | 0.38 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 10 | 0.38 | 0.15 | 0.38 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 10 | 0.38 | 0.15 | 0.38 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 10 | 0.38 | 0.15 | 0.38 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 10 | 0.38 | 0.15 | 0.38 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 10 | 0.38 | 0.15 | 0.38 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 10 | 0.37 | 0.25 | 0.32 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 10 | 0.36 | 0.09 | 0.34 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 10 | 0.36 | 0.28 | 0.24 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 10 | 0.36 | 0.28 | 0.24 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 10 | 0.36 | 0.28 | 0.24 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 10 | 0.35 | 0.17 | 0.36 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 10 | 0.35 | 0.17 | 0.36 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 10 | 0.35 | 0.17 | 0.36 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 10 | 0.34 | 0.21 | 0.3 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 10 | 0.34 | 0.21 | 0.3 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 10 | 0.34 | 0.21 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 10 | 0.34 | 0.09 | 0.33 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 10 | 0.34 | 0.09 | 0.33 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 10 | 0.33 | 0.27 | 0.24 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 10 | 0.29 | 0.26 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 10 | 0.29 | 0.26 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 10 | 0.29 | 0.26 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 10 | 0.29 | 0.26 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 10 | 0.29 | 0.26 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 10 | 0.29 | 0.26 | 0.18 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 10 | 0.29 | 0.09 | 0.31 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 10 | 0.29 | 0.09 | 0.31 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 10 | 0.28 | 0.13 | 0.26 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 10 | 0.28 | 0.13 | 0.26 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 10 | 0.28 | 0.13 | 0.26 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 10 | 0.28 | 0.13 | 0.26 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 10 | 0.28 | 0.13 | 0.26 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 10 | 0.28 | 0.13 | 0.26 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 10 | 0.28 | 0.11 | 0.26 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 10 | 0.28 | 0.11 | 0.26 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 10 | 0.28 | 0.11 | 0.26 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 10 | 0.27 | 0.17 | 0.18 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 10 | 0.27 | 0.04 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 10 | 0.27 | 0.04 | 0.24 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 10 | 0.25 | 0.07 | 0.29 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 10 | 0.25 | 0.07 | 0.29 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 10 | 0.25 | 0.07 | 0.29 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 10 | 0.25 | 0.07 | 0.29 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 10 | 0.23 | 0.1 | 0.22 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 10 | 0.21 | 0.06 | 0.2 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 10 | 0.19 | 0.07 | 0.18 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 10 | 0.19 | 0.07 | 0.18 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 10 | 0.17 | 0.09 | 0.15 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 10 | 0.17 | 0.08 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 10 | 0.17 | 0.08 | 0.14 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 10 | 0.16 | 0.02 | 0.16 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 10 | 0.15 | 0.04 | 0.14 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 10 | 0.15 | 0.04 | 0.14 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 10 | 0.15 | 0.04 | 0.14 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 10 | 0.14 | 0.02 | 0.14 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 10 | 0.14 | 0.04 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 10 | 0.14 | 0.04 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 10 | 0.14 | 0.04 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 10 | 0.14 | 0.04 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 10 | 0.14 | 0.04 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 10 | 0.14 | 0.04 | 0.12 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 10 | 0.14 | 0.03 | 0.13 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 10 | 0.14 | 0.03 | 0.13 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 9 | 0.6 | 0.39 | 0.56 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 9 | 0.6 | 0.39 | 0.56 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 9 | 0.6 | 0.39 | 0.56 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 9 | 0.58 | 0.22 | 0.65 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 9 | 0.58 | 0.22 | 0.65 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 9 | 0.58 | 0.31 | 0.73 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 9 | 0.58 | 0.31 | 0.73 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 9 | 0.58 | 0.31 | 0.73 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 9 | 0.54 | 0.3 | 0.64 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 9 | 0.54 | 0.37 | 0.4 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 9 | 0.53 | 0.42 | 0.32 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 9 | 0.48 | 0.13 | 0.52 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 9 | 0.44 | 0.17 | 0.42 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 9 | 0.41 | 0.19 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 9 | 0.41 | 0.19 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 9 | 0.41 | 0.19 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 9 | 0.41 | 0.19 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 9 | 0.41 | 0.19 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 9 | 0.41 | 0.19 | 0.3 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 9 | 0.4 | 0.13 | 0.42 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 9 | 0.4 | 0.29 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 9 | 0.4 | 0.29 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 9 | 0.4 | 0.29 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 9 | 0.4 | 0.29 | 0.32 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 9 | 0.37 | 0.36 | 0.23 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 9 | 0.33 | 0.11 | 0.34 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 9 | 0.31 | 0.13 | 0.31 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 9 | 0.31 | 0.13 | 0.31 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 9 | 0.31 | 0.13 | 0.31 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 9 | 0.3 | 0.15 | 0.32 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 9 | 0.3 | 0.08 | 0.27 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 9 | 0.29 | 0.06 | 0.31 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 9 | 0.28 | 0.07 | 0.29 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 9 | 0.28 | 0.07 | 0.29 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 9 | 0.28 | 0.11 | 0.22 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 9 | 0.28 | 0.11 | 0.32 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 9 | 0.28 | 0.11 | 0.32 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 9 | 0.28 | 0.1 | 0.25 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 9 | 0.28 | 0.1 | 0.25 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 9 | 0.28 | 0.06 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 9 | 0.28 | 0.06 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 9 | 0.28 | 0.06 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 9 | 0.28 | 0.06 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 9 | 0.28 | 0.06 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 9 | 0.28 | 0.06 | 0.27 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 9 | 0.25 | 0.11 | 0.25 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 9 | 0.25 | 0.11 | 0.25 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 9 | 0.25 | 0.11 | 0.25 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 9 | 0.23 | 0.11 | 0.2 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 9 | 0.23 | 0.03 | 0.23 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 9 | 0.2 | 0.11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 9 | 0.2 | 0.11 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 9 | 0.2 | 0.11 | 0.15 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 9 | 0.2 | 0.06 | 0.19 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 9 | 0.18 | 0.06 | 0.17 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 9 | 0.18 | 0.06 | 0.17 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 9 | 0.18 | 0.06 | 0.17 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 9 | 0.17 | 0.05 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 9 | 0.17 | 0.05 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 9 | 0.17 | 0.05 | 0.16 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 9 | 0.17 | 0.04 | 0.17 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 9 | 0.17 | 0.04 | 0.18 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 9 | 0.16 | 0.06 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 9 | 0.16 | 0.06 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 9 | 0.16 | 0.06 | 0.14 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 9 | 0.15 | 0.04 | 0.14 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 9 | 0.15 | 0.04 | 0.14 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 9 | 0.14 | 0.03 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 9 | 0.14 | 0.03 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 9 | 0.14 | 0.03 | 0.13 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 9 | 0.14 | 0.02 | 0.14 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 9 | 0.14 | 0.02 | 0.14 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 9 | 0.14 | 0.02 | 0.14 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 8 | 2.11 | 1.24 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 8 | 2.11 | 1.24 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 8 | 2.11 | 1.24 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 8 | 2.11 | 1.24 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 8 | 2.11 | 1.24 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 8 | 2.11 | 1.24 | 1.27 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 8 | 1.49 | 1.05 | 0.89 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 8 | 1.49 | 1.05 | 0.89 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 8 | 1.37 | 0.9 | 1.4 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 8 | 1.37 | 0.9 | 1.4 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 8 | 1.37 | 0.9 | 1.4 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 8 | 1.27 | 0.35 | 1.18 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 8 | 1.27 | 0.35 | 1.18 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 8 | 1.12 | 0.03 | 1.1 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 8 | 0.93 | 0.03 | 0.94 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 8 | 0.93 | 0.03 | 0.94 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 8 | 0.93 | 0.03 | 0.94 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 8 | 0.8 | 0.36 | 0.76 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 8 | 0.8 | 0.36 | 0.76 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 8 | 0.76 | 0.57 | 0.61 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 8 | 0.64 | 0.44 | 0.49 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 8 | 0.64 | 0.44 | 0.49 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 8 | 0.6 | 0.32 | 0.52 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 8 | 0.6 | 0.32 | 0.52 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 8 | 0.6 | 0.32 | 0.52 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 8 | 0.51 | 0.3 | 0.42 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 8 | 0.51 | 0.17 | 0.6 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 8 | 0.51 | 0.17 | 0.6 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 8 | 0.44 | 0.23 | 0.37 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 8 | 0.44 | 0.23 | 0.37 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 8 | 0.43 | 0.23 | 0.43 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 8 | 0.41 | 0.23 | 0.36 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 8 | 0.37 | 0.1 | 0.41 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 8 | 0.36 | 0.18 | 0.32 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 8 | 0.36 | 0.18 | 0.32 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 8 | 0.36 | 0.18 | 0.32 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 8 | 0.36 | 0.09 | 0.38 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 8 | 0.36 | 0.09 | 0.38 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 8 | 0.34 | 0.18 | 0.28 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 8 | 0.34 | 0.19 | 0.26 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 8 | 0.31 | 0.15 | 0.29 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 8 | 0.31 | 0.2 | 0.23 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 8 | 0.31 | 0.2 | 0.23 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 8 | 0.31 | 0.2 | 0.23 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 8 | 0.29 | 0.15 | 0.24 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 8 | 0.29 | 0.15 | 0.24 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 8 | 0.29 | 0.15 | 0.24 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 8 | 0.28 | 0.13 | 0.23 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 8 | 0.28 | 0.13 | 0.23 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 8 | 0.28 | 0.13 | 0.23 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 8 | 0.28 | 0.22 | 0.17 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 8 | 0.28 | 0.22 | 0.17 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 8 | 0.28 | 0.22 | 0.17 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 8 | 0.26 | 0.14 | 0.19 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 8 | 0.26 | 0.14 | 0.19 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 8 | 0.26 | 0.14 | 0.19 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 8 | 0.26 | 0.14 | 0.19 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 8 | 0.26 | 0.14 | 0.19 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 8 | 0.26 | 0.14 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 8 | 0.25 | 0.06 | 0.26 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 8 | 0.23 | 0.1 | 0.18 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 8 | 0.23 | 0.1 | 0.18 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 8 | 0.22 | 0.07 | 0.2 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 8 | 0.22 | 0.15 | 0.14 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 8 | 0.22 | 0.15 | 0.14 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 8 | 0.22 | 0.15 | 0.14 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 8 | 0.2 | 0.07 | 0.19 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 8 | 0.2 | 0.07 | 0.19 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 8 | 0.2 | 0.06 | 0.2 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 8 | 0.2 | 0.06 | 0.2 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 8 | 0.2 | 0.06 | 0.2 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 8 | 0.18 | 0.09 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 8 | 0.18 | 0.09 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 8 | 0.18 | 0.09 | 0.15 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 8 | 0.18 | 0.06 | 0.16 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 8 | 0.18 | 0.04 | 0.17 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 8 | 0.17 | 0.12 | 0.13 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 8 | 0.17 | 0.06 | 0.15 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 8 | 0.17 | 0.06 | 0.16 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 8 | 0.16 | 0.06 | 0.13 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 8 | 0.15 | 0.03 | 0.15 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 8 | 0.14 | 0.03 | 0.14 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 8 | 0.14 | 0.02 | 0.16 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 7 | 1.22 | 0.71 | 1.0 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 7 | 1.22 | 0.71 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 7 | 1.22 | 0.71 | 1.0 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 7 | 1.13 | 0.85 | 0.67 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 7 | 1.13 | 0.85 | 0.67 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 7 | 1.13 | 0.85 | 0.67 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 7 | 0.99 | 0.49 | 1.16 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 7 | 0.99 | 0.49 | 1.16 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 7 | 0.96 | 1.07 | 0.25 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 7 | 0.96 | 1.07 | 0.25 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 7 | 0.85 | 0.44 | 0.86 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 7 | 0.85 | 0.44 | 0.86 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 7 | 0.81 | 0.11 | 0.83 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 7 | 0.81 | 0.11 | 0.83 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 7 | 0.75 | 0.33 | 0.87 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 7 | 0.75 | 0.33 | 0.87 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 7 | 0.75 | 0.11 | 0.71 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 7 | 0.75 | 0.11 | 0.71 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 7 | 0.75 | 0.11 | 0.71 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 7 | 0.75 | 0.11 | 0.71 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 7 | 0.68 | 0.44 | 0.71 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 7 | 0.55 | 0.28 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 7 | 0.55 | 0.28 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 7 | 0.55 | 0.28 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 7 | 0.55 | 0.28 | 0.49 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 7 | 0.53 | 0.21 | 0.6 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 7 | 0.53 | 0.21 | 0.6 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 7 | 0.53 | 0.26 | 0.6 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 7 | 0.49 | 0.16 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 7 | 0.49 | 0.16 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 7 | 0.49 | 0.16 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 7 | 0.49 | 0.16 | 0.47 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 7 | 0.46 | 0.17 | 0.38 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 7 | 0.46 | 0.17 | 0.38 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 7 | 0.44 | 0.11 | 0.43 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 7 | 0.39 | 0.15 | 0.36 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 7 | 0.39 | 0.15 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 7 | 0.38 | 0.31 | 0.27 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 7 | 0.38 | 0.31 | 0.27 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 7 | 0.38 | 0.31 | 0.27 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 7 | 0.38 | 0.27 | 0.26 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 7 | 0.38 | 0.27 | 0.26 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 7 | 0.34 | 0.2 | 0.3 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 7 | 0.34 | 0.2 | 0.3 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 7 | 0.34 | 0.2 | 0.3 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 7 | 0.33 | 0.09 | 0.33 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 7 | 0.33 | 0.09 | 0.33 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 7 | 0.31 | 0.08 | 0.33 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 7 | 0.3 | 0.15 | 0.27 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 7 | 0.3 | 0.15 | 0.27 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 7 | 0.3 | 0.15 | 0.27 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 7 | 0.28 | 0.11 | 0.28 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 7 | 0.28 | 0.11 | 0.28 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 7 | 0.28 | 0.11 | 0.28 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 7 | 0.28 | 0.14 | 0.22 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 7 | 0.28 | 0.14 | 0.22 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 7 | 0.28 | 0.14 | 0.22 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 7 | 0.28 | 0.14 | 0.22 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 7 | 0.28 | 0.14 | 0.22 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 7 | 0.28 | 0.14 | 0.22 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 7 | 0.27 | 0.16 | 0.19 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 7 | 0.27 | 0.16 | 0.19 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 7 | 0.27 | 0.09 | 0.3 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 7 | 0.27 | 0.09 | 0.3 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 7 | 0.27 | 0.09 | 0.27 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 7 | 0.27 | 0.09 | 0.27 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 7 | 0.27 | 0.09 | 0.27 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 7 | 0.27 | 0.14 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 7 | 0.27 | 0.14 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 7 | 0.27 | 0.14 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 7 | 0.27 | 0.14 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 7 | 0.27 | 0.14 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 7 | 0.27 | 0.14 | 0.2 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 7 | 0.26 | 0.17 | 0.22 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 7 | 0.26 | 0.13 | 0.2 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 7 | 0.26 | 0.13 | 0.2 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 7 | 0.26 | 0.13 | 0.2 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 7 | 0.24 | 0.09 | 0.23 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 7 | 0.24 | 0.09 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 7 | 0.24 | 0.09 | 0.23 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 7 | 0.24 | 0.09 | 0.23 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 7 | 0.24 | 0.09 | 0.23 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 7 | 0.24 | 0.09 | 0.23 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 7 | 0.22 | 0.11 | 0.16 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 7 | 0.22 | 0.11 | 0.16 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 7 | 0.2 | 0.09 | 0.17 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 7 | 0.2 | 0.09 | 0.17 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 7 | 0.2 | 0.09 | 0.17 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 7 | 0.19 | 0.04 | 0.19 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 7 | 0.18 | 0.06 | 0.18 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 7 | 0.18 | 0.06 | 0.18 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 7 | 0.18 | 0.06 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 7 | 0.17 | 0.04 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 7 | 0.17 | 0.04 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 7 | 0.17 | 0.04 | 0.18 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 7 | 0.17 | 0.04 | 0.18 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 7 | 0.17 | 0.04 | 0.18 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 7 | 0.17 | 0.04 | 0.18 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 7 | 0.17 | 0.03 | 0.16 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 7 | 0.17 | 0.03 | 0.16 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 7 | 0.17 | 0.03 | 0.16 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 7 | 0.16 | 0.06 | 0.15 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 7 | 0.16 | 0.05 | 0.14 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 7 | 0.15 | 0.04 | 0.13 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 7 | 0.15 | 0.03 | 0.16 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 7 | 0.13 | 0.01 | 0.13 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 6 | 1.19 | 0.72 | 0.98 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 6 | 1.19 | 0.72 | 0.98 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 6 | 1.19 | 0.72 | 0.98 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 6 | 0.97 | 0.48 | 1.21 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 6 | 0.97 | 0.48 | 1.21 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 6 | 0.9 | 0.58 | 0.82 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 6 | 0.9 | 0.58 | 0.82 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 6 | 0.9 | 0.58 | 0.82 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 6 | 0.86 | 0.83 | 0.65 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 6 | 0.86 | 0.83 | 0.65 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 6 | 0.84 | 0.16 | 0.83 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 6 | 0.84 | 0.16 | 0.83 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 6 | 0.84 | 0.16 | 0.83 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 6 | 0.77 | 0.32 | 0.82 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 6 | 0.77 | 0.32 | 0.82 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 6 | 0.74 | 0.61 | 0.62 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 6 | 0.74 | 0.61 | 0.62 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 6 | 0.64 | 0.28 | 0.68 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 6 | 0.64 | 0.28 | 0.68 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 6 | 0.64 | 0.28 | 0.68 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 6 | 0.64 | 0.28 | 0.68 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 6 | 0.64 | 0.28 | 0.68 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 6 | 0.64 | 0.28 | 0.68 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 6 | 0.56 | 0.32 | 0.43 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 6 | 0.56 | 0.32 | 0.43 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 6 | 0.5 | 0.23 | 0.47 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 6 | 0.49 | 0.04 | 0.5 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 6 | 0.47 | 0.18 | 0.42 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 6 | 0.47 | 0.18 | 0.42 |
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 6 | 0.47 | 0.18 | 0.42 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 6 | 0.47 | 0.18 | 0.42 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 6 | 0.47 | 0.18 | 0.42 |
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 6 | 0.47 | 0.18 | 0.42 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 6 | 0.44 | 0.27 | 0.34 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 6 | 0.44 | 0.27 | 0.34 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 6 | 0.44 | 0.27 | 0.34 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 6 | 0.41 | 0.2 | 0.38 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 6 | 0.41 | 0.2 | 0.38 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 6 | 0.4 | 0.09 | 0.38 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 6 | 0.38 | 0.25 | 0.33 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 6 | 0.37 | 0.17 | 0.38 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 6 | 0.37 | 0.14 | 0.38 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 6 | 0.37 | 0.14 | 0.38 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 6 | 0.36 | 0.09 | 0.38 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 6 | 0.36 | 0.09 | 0.38 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 6 | 0.35 | 0.16 | 0.28 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 6 | 0.35 | 0.16 | 0.28 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 6 | 0.35 | 0.16 | 0.28 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 6 | 0.35 | 0.16 | 0.28 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 6 | 0.35 | 0.16 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 6 | 0.35 | 0.16 | 0.28 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 6 | 0.32 | 0.21 | 0.25 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 6 | 0.31 | 0.15 | 0.32 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 6 | 0.3 | 0.17 | 0.24 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 6 | 0.3 | 0.17 | 0.24 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 6 | 0.3 | 0.17 | 0.24 |
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 6 | 0.3 | 0.13 | 0.3 |
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 6 | 0.3 | 0.13 | 0.3 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 6 | 0.3 | 0.13 | 0.3 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 6 | 0.28 | 0.09 | 0.26 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 6 | 0.28 | 0.09 | 0.26 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 6 | 0.28 | 0.09 | 0.26 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 6 | 0.28 | 0.14 | 0.28 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 6 | 0.28 | 0.14 | 0.28 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 6 | 0.28 | 0.1 | 0.28 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 6 | 0.28 | 0.1 | 0.28 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 6 | 0.28 | 0.1 | 0.28 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 6 | 0.27 | 0.12 | 0.28 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 6 | 0.26 | 0.06 | 0.28 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 6 | 0.26 | 0.06 | 0.28 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 6 | 0.26 | 0.25 | 0.14 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 6 | 0.25 | 0.09 | 0.24 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 6 | 0.25 | 0.09 | 0.24 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 6 | 0.25 | 0.09 | 0.24 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 6 | 0.25 | 0.09 | 0.24 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 6 | 0.25 | 0.09 | 0.24 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 6 | 0.25 | 0.09 | 0.24 |
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 6 | 0.24 | 0.13 | 0.2 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 6 | 0.23 | 0.07 | 0.2 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 6 | 0.23 | 0.07 | 0.2 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 6 | 0.23 | 0.07 | 0.2 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 6 | 0.22 | 0.09 | 0.2 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 6 | 0.22 | 0.09 | 0.2 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 6 | 0.22 | 0.09 | 0.2 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 6 | 0.22 | 0.09 | 0.2 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 6 | 0.22 | 0.09 | 0.2 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 6 | 0.22 | 0.09 | 0.2 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 6 | 0.19 | 0.04 | 0.2 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 6 | 0.19 | 0.04 | 0.2 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 6 | 0.19 | 0.08 | 0.16 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 6 | 0.19 | 0.08 | 0.16 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 6 | 0.19 | 0.08 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 6 | 0.19 | 0.08 | 0.16 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 6 | 0.19 | 0.08 | 0.16 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 6 | 0.19 | 0.08 | 0.16 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 6 | 0.18 | 0.05 | 0.16 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 6 | 0.18 | 0.06 | 0.16 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 6 | 0.18 | 0.01 | 0.18 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 6 | 0.15 | 0.04 | 0.15 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 6 | 0.14 | 0.04 | 0.12 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 6 | 0.14 | 0.04 | 0.12 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 6 | 0.13 | 0.03 | 0.12 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 6 | 0.13 | 0.03 | 0.12 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 6 | 0.13 | 0.03 | 0.12 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 6 | 0.13 | 0.03 | 0.12 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 6 | 0.12 | 0.01 | 0.12 |
| (1,20) | 1:47:A:THR:HG21 | 1:50:A:LEU:HA | 5 | 1.44 | 0.65 | 1.53 |
| (1,20) | 1:47:A:THR:HG22 | 1:50:A:LEU:HA | 5 | 1.44 | 0.65 | 1.53 |
| (1,20) | 1:47:A:THR:HG23 | 1:50:A:LEU:HA | 5 | 1.44 | 0.65 | 1.53 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG21 | 5 | 1.17 | 0.21 | 1.12 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG22 | 5 | 1.17 | 0.21 | 1.12 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG23 | 5 | 1.17 | 0.21 | 1.12 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG21 | 5 | 1.17 | 0.21 | 1.12 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG22 | 5 | 1.17 | 0.21 | 1.12 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG23 | 5 | 1.17 | 0.21 | 1.12 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG21 | 5 | 1.0 | 0.05 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG22 | 5 | 1.0 | 0.05 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG23 | 5 | 1.0 | 0.05 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG21 | 5 | 1.0 | 0.05 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG22 | 5 | 1.0 | 0.05 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG23 | 5 | 1.0 | 0.05 | 1.01 |
| (1,232) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 5 | 0.97 | 0.54 | 0.73 |
| (1,12) | 1:47:A:THR:HB | 1:50:A:LEU:HG | 5 | 0.94 | 0.38 | 1.1 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG21 | 5 | 0.91 | 0.77 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG22 | 5 | 0.91 | 0.77 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG23 | 5 | 0.91 | 0.77 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG21 | 5 | 0.91 | 0.77 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG22 | 5 | 0.91 | 0.77 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG23 | 5 | 0.91 | 0.77 | 0.68 |
| (1,468) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 5 | 0.89 | 0.19 | 0.81 |
| (1,613) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG2 | 5 | 0.86 | 0.41 | 0.88 |
| (1,613) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG2 | 5 | 0.86 | 0.41 | 0.88 |
| (1,613) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG2 | 5 | 0.86 | 0.41 | 0.88 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 5 | 0.79 | 0.32 | 0.78 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 5 | 0.79 | 0.32 | 0.78 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 5 | 0.77 | 0.22 | 0.66 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 5 | 0.77 | 0.22 | 0.66 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 5 | 0.77 | 0.22 | 0.66 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 5 | 0.69 | 0.3 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 5 | 0.69 | 0.3 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 5 | 0.69 | 0.3 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 5 | 0.69 | 0.3 | 0.59 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 5 | 0.68 | 0.31 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 5 | 0.68 | 0.31 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 5 | 0.68 | 0.31 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 5 | 0.68 | 0.31 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 5 | 0.68 | 0.31 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 5 | 0.68 | 0.31 | 0.64 |
| (1,3079) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 5 | 0.65 | 0.49 | 0.61 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 5 | 0.59 | 0.37 | 0.41 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 5 | 0.59 | 0.37 | 0.41 |
| (1,1002) | 1:123:A:LYS:HD3 | 1:136:A:TYR:HB3 | 5 | 0.58 | 0.66 | 0.21 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD11 | 5 | 0.54 | 0.23 | 0.38 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD12 | 5 | 0.54 | 0.23 | 0.38 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD13 | 5 | 0.54 | 0.23 | 0.38 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD11 | 5 | 0.49 | 0.2 | 0.35 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD12 | 5 | 0.49 | 0.2 | 0.35 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD13 | 5 | 0.49 | 0.2 | 0.35 |
| (1,609) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 5 | 0.46 | 0.29 | 0.39 |
| (1,609) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 5 | 0.46 | 0.29 | 0.39 |
| (1,609) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 5 | 0.46 | 0.29 | 0.39 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB2 | 5 | 0.45 | 0.1 | 0.42 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB3 | 5 | 0.45 | 0.1 | 0.42 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB2 | 5 | 0.45 | 0.1 | 0.42 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB3 | 5 | 0.45 | 0.1 | 0.42 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB2 | 5 | 0.45 | 0.1 | 0.42 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB3 | 5 | 0.45 | 0.1 | 0.42 |
| (1,3474) | 2:17:B:LYS:HD2 | 2:18:B:CYS:H | 5 | 0.43 | 0.18 | 0.39 |
| (1,3474) | 2:17:B:LYS:HD3 | 2:18:B:CYS:H | 5 | 0.43 | 0.18 | 0.39 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB1 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB2 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB3 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB1 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB2 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB3 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB1 | 5 | 0.42 | 0.22 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB2 | 5 | 0.42 | 0.22 | 0.29 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB3 | 5 | 0.42 | 0.22 | 0.29 |
| (1,183) | 1:58:A:HIS:HB3 | 2:12:B:ASN:HD22 | 5 | 0.42 | 0.18 | 0.4 |
| (1,1731) | 1:167:A:ASP:HA | 1:196:A:ASN:HB3 | 5 | 0.4 | 0.2 | 0.37 |
| (1,3248) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HE1 | 5 | 0.39 | 0.2 | 0.26 |
| (1,3248) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HE1 | 5 | 0.39 | 0.2 | 0.26 |
| (1,3248) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HE1 | 5 | 0.39 | 0.2 | 0.26 |
| (1,3116) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HA | 5 | 0.39 | 0.16 | 0.39 |
| (1,3116) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HA | 5 | 0.39 | 0.16 | 0.39 |
| (1,3204) | 1:88:A:GLN:HB3 | 1:90:A:HIS:HE1 | 5 | 0.36 | 0.26 | 0.19 |
| (1,3990) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 5 | 0.36 | 0.14 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 5 | 0.36 | 0.14 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 5 | 0.36 | 0.14 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 5 | 0.36 | 0.14 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 5 | 0.36 | 0.14 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 5 | 0.36 | 0.14 | 0.34 |
| (1,2437) | 1:82:A:LEU:HG | 1:113:A:ASP:H | 5 | 0.35 | 0.15 | 0.34 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG11 | 5 | 0.34 | 0.15 | 0.4 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG12 | 5 | 0.34 | 0.15 | 0.4 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG13 | 5 | 0.34 | 0.15 | 0.4 |
| (1,676) | 1:103:A:THR:HG21 | 1:128:A:LEU:H | 5 | 0.33 | 0.2 | 0.27 |
| (1,676) | 1:103:A:THR:HG22 | 1:128:A:LEU:H | 5 | 0.33 | 0.2 | 0.27 |
| (1,676) | 1:103:A:THR:HG23 | 1:128:A:LEU:H | 5 | 0.33 | 0.2 | 0.27 |
| (1,348) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HB2 | 5 | 0.33 | 0.21 | 0.26 |
| (1,348) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HB2 | 5 | 0.33 | 0.21 | 0.26 |
| (1,348) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HB2 | 5 | 0.33 | 0.21 | 0.26 |
| (1,2303) | 1:77:A:GLN:HB2 | 1:80:A:SER:H | 5 | 0.33 | 0.19 | 0.2 |
| (1,3091) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 5 | 0.31 | 0.22 | 0.22 |
| (1,3208) | 1:126:A:ALA:HB1 | 1:133:A:TRP:HD1 | 5 | 0.31 | 0.12 | 0.28 |
| (1,3208) | 1:126:A:ALA:HB2 | 1:133:A:TRP:HD1 | 5 | 0.31 | 0.12 | 0.28 |
| (1,3208) | 1:126:A:ALA:HB3 | 1:133:A:TRP:HD1 | 5 | 0.31 | 0.12 | 0.28 |
| (1,3396) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HA | 5 | 0.31 | 0.11 | 0.31 |
| (1,3396) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HA | 5 | 0.31 | 0.11 | 0.31 |
| (1,3396) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HA | 5 | 0.31 | 0.11 | 0.31 |
| (1,3682) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 5 | 0.3 | 0.01 | 0.3 |
| (1,3682) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 5 | 0.3 | 0.01 | 0.3 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 5 | 0.29 | 0.07 | 0.31 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB3 | 5 | 0.29 | 0.07 | 0.31 |
| (1,2761) | 1:167:A:ASP:H | 1:196:A:ASN:HB2 | 5 | 0.29 | 0.05 | 0.28 |
| (1,3479) | 1:53:A:THR:HG21 | 2:9:B:ILE:HB | 5 | 0.29 | 0.19 | 0.2 |
| (1,3479) | 1:53:A:THR:HG22 | 2:9:B:ILE:HB | 5 | 0.29 | 0.19 | 0.2 |
| (1,3479) | 1:53:A:THR:HG23 | 2:9:B:ILE:HB | 5 | 0.29 | 0.19 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2765) | 1:168:A:ALA:H | 1:196:A:ASN:HA | 5 | 0.28 | 0.17 | 0.27 |
| (1,1321) | 1:158:A:ASP:HB2 | 1:162:A:THR:HA | 5 | 0.28 | 0.1 | 0.27 |
| (1,2544) | 1:128:A:LEU:HD11 | 1:131:A:LYS:H | 5 | 0.28 | 0.11 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD12 | 1:131:A:LYS:H | 5 | 0.28 | 0.11 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD13 | 1:131:A:LYS:H | 5 | 0.28 | 0.11 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD21 | 1:131:A:LYS:H | 5 | 0.28 | 0.11 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD22 | 1:131:A:LYS:H | 5 | 0.28 | 0.11 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD23 | 1:131:A:LYS:H | 5 | 0.28 | 0.11 | 0.34 |
| (1,2002) | 1:216:A:LEU:H | 1:216:A:LEU:HG | 5 | 0.27 | 0.03 | 0.28 |
| (1,2506) | 1:147:A:GLY:HA2 | 1:179:A:LEU:H | 5 | 0.24 | 0.07 | 0.23 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG11 | 5 | 0.23 | 0.16 | 0.16 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG12 | 5 | 0.23 | 0.16 | 0.16 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG13 | 5 | 0.23 | 0.16 | 0.16 |
| (1,2074) | 1:223:A:THR:HB | 1:224:A:LEU:H | 5 | 0.23 | 0.02 | 0.22 |
| (1,3521) | 1:59:A:ALA:HB1 | 2:12:B:ASN:HB2 | 5 | 0.22 | 0.1 | 0.17 |
| (1,3521) | 1:59:A:ALA:HB2 | 2:12:B:ASN:HB2 | 5 | 0.22 | 0.1 | 0.17 |
| (1,3521) | 1:59:A:ALA:HB3 | 2:12:B:ASN:HB2 | 5 | 0.22 | 0.1 | 0.17 |
| (1,2120) | 1:74:A:ASP:HA | 1:83:A:GLN:HG3 | 5 | 0.21 | 0.09 | 0.22 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB1 | 5 | 0.2 | 0.09 | 0.18 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB2 | 5 | 0.2 | 0.09 | 0.18 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB3 | 5 | 0.2 | 0.09 | 0.18 |
| (1,191) | 1:152:A:LYS:H | 1:168:A:ALA:HA | 5 | 0.2 | 0.08 | 0.17 |
| (1,3411) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB2 | 5 | 0.19 | 0.07 | 0.17 |
| (1,3411) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB2 | 5 | 0.19 | 0.07 | 0.17 |
| (1,3411) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB2 | 5 | 0.19 | 0.07 | 0.17 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD2 | 5 | 0.18 | 0.04 | 0.2 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD3 | 5 | 0.18 | 0.04 | 0.2 |
| (1,776) | 1:113:A:ASP:HA | 1:118:A:ILE:HG12 | 5 | 0.18 | 0.06 | 0.15 |
| (1,2279) | 1:75:A:ILE:H | 1:84:A:ALA:H | 5 | 0.17 | 0.04 | 0.18 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB2 | 5 | 0.17 | 0.06 | 0.16 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB3 | 5 | 0.17 | 0.06 | 0.16 |
| (1,1795) | 1:201:A:ILE:HD11 | 1:202:A:THR:H | 5 | 0.16 | 0.05 | 0.16 |
| (1,1795) | 1:201:A:ILE:HD12 | 1:202:A:THR:H | 5 | 0.16 | 0.05 | 0.16 |
| (1,1795) | 1:201:A:ILE:HD13 | 1:202:A:THR:H | 5 | 0.16 | 0.05 | 0.16 |
| (1,2752) | 1:154:A:ILE:HA | 1:166:A:ASP:H | 5 | 0.16 | 0.05 | 0.13 |
| (1,2288) | 1:75:A:ILE:HB | 1:76:A:MET:H | 5 | 0.16 | 0.04 | 0.14 |
| (1,142) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HB3 | 5 | 0.15 | 0.05 | 0.12 |
| (1,142) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HB3 | 5 | 0.15 | 0.05 | 0.12 |
| (1,142) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HB3 | 5 | 0.15 | 0.05 | 0.12 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE2 | 5 | 0.15 | 0.0 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE3 | 5 | 0.15 | 0.0 | 0.15 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD11 | 5 | 0.13 | 0.03 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD12 | 5 | 0.13 | 0.03 | 0.14 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD13 | 5 | 0.13 | 0.03 | 0.14 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB1 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB2 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB1 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB2 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB1 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB2 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,619) | 1:98:A:PRO:HB2 | 1:99:A:GLU:HA | 5 | 0.11 | 0.01 | 0.11 |
| (1,966) | 1:134:A:VAL:HA | 1:155:A:LYS:HG3 | 5 | 0.11 | 0.01 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE1 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE2 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2122) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 4 | 1.48 | 0.34 | 1.36 |
| (1,615) | 1:94:A:ALA:H | 1:97:A:GLN:HG2 | 4 | 1.39 | 0.4 | 1.31 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD11 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD12 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD13 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD11 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD12 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD13 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD11 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD12 | 4 | 1.19 | 0.12 | 1.15 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD13 | 4 | 1.19 | 0.12 | 1.15 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 4 | 0.98 | 0.42 | 0.94 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 4 | 0.98 | 0.42 | 0.94 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE1 | 4 | 0.96 | 0.33 | 0.86 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE2 | 4 | 0.96 | 0.33 | 0.86 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE3 | 4 | 0.96 | 0.33 | 0.86 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE1 | 4 | 0.96 | 0.33 | 0.86 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE2 | 4 | 0.96 | 0.33 | 0.86 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE3 | 4 | 0.96 | 0.33 | 0.86 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 4 | 0.8 | 0.57 | 0.69 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 4 | 0.8 | 0.57 | 0.69 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 4 | 0.76 | 0.4 | 0.7 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 4 | 0.76 | 0.4 | 0.7 |
| (1,2217) | 1:62:A:ASP:H | 1:66:A:ASP:HB2 | 4 | 0.73 | 0.7 | 0.38 |
| (1,242) | 1:142:A:THR:HG21 | 1:146:A:PRO:HD2 | 4 | 0.73 | 0.57 | 0.72 |
| (1,242) | 1:142:A:THR:HG22 | 1:146:A:PRO:HD2 | 4 | 0.73 | 0.57 | 0.72 |
| (1,242) | 1:142:A:THR:HG23 | 1:146:A:PRO:HD2 | 4 | 0.73 | 0.57 | 0.72 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 4 | 0.7 | 0.51 | 0.64 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 4 | 0.7 | 0.51 | 0.64 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 4 | 0.7 | 0.51 | 0.64 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 4 | 0.7 | 0.51 | 0.64 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 4 | 0.66 | 0.37 | 0.68 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 4 | 0.66 | 0.37 | 0.68 |
| (1,3496) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HA | 4 | 0.66 | 0.43 | 0.55 |
| (1,3496) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HA | 4 | 0.66 | 0.43 | 0.55 |
| (1,3496) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HA | 4 | 0.66 | 0.43 | 0.55 |
| (1,3074) | 1:167:A:ASP:H | 1:196:A:ASN:HD22 | 4 | 0.64 | 0.19 | 0.62 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG2 | 4 | 0.64 | 0.25 | 0.52 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG3 | 4 | 0.64 | 0.25 | 0.52 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD11 | 4 | 0.62 | 0.13 | 0.68 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD12 | 4 | 0.62 | 0.13 | 0.68 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD13 | 4 | 0.62 | 0.13 | 0.68 |
| (1,956) | 1:190:A:LYS:HA | 1:190:A:LYS:HE3 | 4 | 0.6 | 0.02 | 0.6 |
| (1,446) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA3 | 4 | 0.57 | 0.39 | 0.53 |
| (1,446) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA3 | 4 | 0.57 | 0.39 | 0.53 |
| (1,446) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA3 | 4 | 0.57 | 0.39 | 0.53 |
| (1,2375) | 1:92:A:LYS:HG2 | 1:93:A:GLU:H | 4 | 0.56 | 0.19 | 0.54 |
| (1,2375) | 1:92:A:LYS:HG3 | 1:93:A:GLU:H | 4 | 0.56 | 0.19 | 0.54 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG11 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG12 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG13 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG21 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG22 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG23 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG11 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG12 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG13 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG21 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG22 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG23 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG11 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG12 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG13 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG21 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG22 | 4 | 0.55 | 0.13 | 0.54 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG23 | 4 | 0.55 | 0.13 | 0.54 |
| (1,3486) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HA | 4 | 0.5 | 0.24 | 0.58 |
| (1,3486) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HA | 4 | 0.5 | 0.24 | 0.58 |
| (1,3486) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HA | 4 | 0.5 | 0.24 | 0.58 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE2 | 4 | 0.48 | 0.2 | 0.54 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE3 | 4 | 0.48 | 0.2 | 0.54 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE2 | 4 | 0.48 | 0.2 | 0.54 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE3 | 4 | 0.48 | 0.2 | 0.54 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD11 | 4 | 0.48 | 0.23 | 0.51 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD12 | 4 | 0.48 | 0.23 | 0.51 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD13 | 4 | 0.48 | 0.23 | 0.51 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD21 | 4 | 0.46 | 0.15 | 0.4 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD22 | 4 | 0.46 | 0.15 | 0.4 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD21 | 4 | 0.46 | 0.15 | 0.4 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD22 | 4 | 0.46 | 0.15 | 0.4 |
| (1,3488) | 1:54:A:ILE:HD11 | 2:11:B:CYS:H | 4 | 0.46 | 0.18 | 0.52 |
| (1,3488) | 1:54:A:ILE:HD12 | 2:11:B:CYS:H | 4 | 0.46 | 0.18 | 0.52 |
| (1,3488) | 1:54:A:ILE:HD13 | 2:11:B:CYS:H | 4 | 0.46 | 0.18 | 0.52 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG11 | 4 | 0.43 | 0.03 | 0.44 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG12 | 4 | 0.43 | 0.03 | 0.44 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG13 | 4 | 0.43 | 0.03 | 0.44 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG21 | 4 | 0.43 | 0.03 | 0.44 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG22 | 4 | 0.43 | 0.03 | 0.44 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG23 | 4 | 0.43 | 0.03 | 0.44 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD2 | 4 | 0.42 | 0.05 | 0.42 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD3 | 4 | 0.42 | 0.05 | 0.42 |
| (1,2129) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB3 | 4 | 0.41 | 0.41 | 0.2 |
| (1,330) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HA | 4 | 0.4 | 0.18 | 0.33 |
| (1,3605) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HA | 4 | 0.39 | 0.11 | 0.42 |
| (1,3605) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HA | 4 | 0.39 | 0.11 | 0.42 |
| (1,3505) | 1:51:A:PRO:HB3 | 2:7:B:PRO:HD3 | 4 | 0.38 | 0.12 | 0.38 |
| (1,3386) | 2:8:B:ILE:HD11 | 2:9:B:ILE:H | 4 | 0.37 | 0.31 | 0.23 |
| (1,3386) | 2:8:B:ILE:HD12 | 2:9:B:ILE:H | 4 | 0.37 | 0.31 | 0.23 |
| (1,3386) | 2:8:B:ILE:HD13 | 2:9:B:ILE:H | 4 | 0.37 | 0.31 | 0.23 |
| (1,484) | 1:82:A:LEU:HG | 1:83:A:GLN:H | 4 | 0.36 | 0.22 | 0.36 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD21 | 4 | 0.35 | 0.17 | 0.29 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD22 | 4 | 0.35 | 0.17 | 0.29 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD23 | 4 | 0.35 | 0.17 | 0.29 |
| (1,591) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 4 | 0.31 | 0.03 | 0.32 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG21 | 4 | 0.3 | 0.09 | 0.27 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG22 | 4 | 0.3 | 0.09 | 0.27 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG23 | 4 | 0.3 | 0.09 | 0.27 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG21 | 4 | 0.3 | 0.09 | 0.27 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG22 | 4 | 0.3 | 0.09 | 0.27 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG23 | 4 | 0.3 | 0.09 | 0.27 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG21 | 4 | 0.3 | 0.17 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG22 | 4 | 0.3 | 0.17 | 0.28 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG23 | 4 | 0.3 | 0.17 | 0.28 |
| (1,1963) | 1:161:A:LYS:HD2 | 1:189:A:VAL:H | 4 | 0.29 | 0.21 | 0.21 |
| (1,1963) | 1:161:A:LYS:HD3 | 1:189:A:VAL:H | 4 | 0.29 | 0.21 | 0.21 |
| (1,65) | 1:52:A:VAL:HG11 | 1:76:A:MET:H | 4 | 0.28 | 0.12 | 0.29 |
| (1,65) | 1:52:A:VAL:HG12 | 1:76:A:MET:H | 4 | 0.28 | 0.12 | 0.29 |
| (1,65) | 1:52:A:VAL:HG13 | 1:76:A:MET:H | 4 | 0.28 | 0.12 | 0.29 |
| (1,3274) | 1:111:A:HIS:HD2 | 1:113:A:ASP:H | 4 | 0.27 | 0.13 | 0.25 |
| (1,1111) | 1:116:A:GLN:HA | 1:142:A:THR:HA | 4 | 0.27 | 0.1 | 0.28 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD2 | 4 | 0.26 | 0.07 | 0.24 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD3 | 4 | 0.26 | 0.07 | 0.24 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD2 | 4 | 0.26 | 0.07 | 0.24 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD3 | 4 | 0.26 | 0.07 | 0.24 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD2 | 4 | 0.26 | 0.07 | 0.24 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD3 | 4 | 0.26 | 0.07 | 0.24 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG11 | 4 | 0.26 | 0.11 | 0.24 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG12 | 4 | 0.26 | 0.11 | 0.24 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG13 | 4 | 0.26 | 0.11 | 0.24 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG11 | 4 | 0.26 | 0.11 | 0.24 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG12 | 4 | 0.26 | 0.11 | 0.24 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG13 | 4 | 0.26 | 0.11 | 0.24 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD1 | 4 | 0.25 | 0.14 | 0.21 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD2 | 4 | 0.25 | 0.14 | 0.21 |
| (1,3277) | 1:69:A:PHE:HD1 | 1:87:A:VAL:HB | 4 | 0.24 | 0.15 | 0.19 |
| (1,3277) | 1:69:A:PHE:HD2 | 1:87:A:VAL:HB | 4 | 0.24 | 0.15 | 0.19 |
| (1,3538) | 1:48:A:ASN:HD21 | 1:49:A:ASP:H | 4 | 0.23 | 0.08 | 0.2 |
| (1,3538) | 1:48:A:ASN:HD22 | 1:49:A:ASP:H | 4 | 0.23 | 0.08 | 0.2 |
| (1,893) | 1:155:A:LYS:HE3 | 1:166:A:ASP:H | 4 | 0.22 | 0.12 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD11 | 4 | 0.22 | 0.1 | 0.2 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD12 | 4 | 0.22 | 0.1 | 0.2 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD13 | 4 | 0.22 | 0.1 | 0.2 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD21 | 4 | 0.22 | 0.1 | 0.2 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD22 | 4 | 0.22 | 0.1 | 0.2 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD23 | 4 | 0.22 | 0.1 | 0.2 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD2 | 4 | 0.21 | 0.05 | 0.19 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD3 | 4 | 0.21 | 0.05 | 0.19 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD21 | 4 | 0.21 | 0.07 | 0.2 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD22 | 4 | 0.21 | 0.07 | 0.2 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD23 | 4 | 0.21 | 0.07 | 0.2 |
| (1,1146) | 1:142:A:THR:HA | 1:147:A:GLY:HA3 | 4 | 0.21 | 0.06 | 0.18 |
| (1,564) | 1:74:A:ASP:HA | 1:75:A:ILE:HB | 4 | 0.21 | 0.06 | 0.22 |
| (1,33) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB3 | 4 | 0.2 | 0.05 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,33) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB3 | 4 | 0.2 | 0.05 | 0.19 |
| (1,33) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB3 | 4 | 0.2 | 0.05 | 0.19 |
| (1,1713) | 1:194:A:ILE:HG21 | 1:195:A:ASN:HA | 4 | 0.2 | 0.04 | 0.2 |
| (1,1713) | 1:194:A:ILE:HG22 | 1:195:A:ASN:HA | 4 | 0.2 | 0.04 | 0.2 |
| (1,1713) | 1:194:A:ILE:HG23 | 1:195:A:ASN:HA | 4 | 0.2 | 0.04 | 0.2 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE2 | 4 | 0.2 | 0.08 | 0.18 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE3 | 4 | 0.2 | 0.08 | 0.18 |
| (1,17) | 1:47:A:THR:HG21 | 1:48:A:ASN:H | 4 | 0.19 | 0.06 | 0.16 |
| (1,17) | 1:47:A:THR:HG22 | 1:48:A:ASN:H | 4 | 0.19 | 0.06 | 0.16 |
| (1,17) | 1:47:A:THR:HG23 | 1:48:A:ASN:H | 4 | 0.19 | 0.06 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD11 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD12 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD13 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD11 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD12 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD13 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD11 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD12 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD13 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD11 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD12 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD13 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD11 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD12 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD13 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD11 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD12 | 4 | 0.19 | 0.08 | 0.16 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD13 | 4 | 0.19 | 0.08 | 0.16 |
| (1,3229) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD21 | 4 | 0.19 | 0.05 | 0.16 |
| (1,769) | 1:82:A:LEU:HG | 1:112:A:TYR:HA | 4 | 0.18 | 0.08 | 0.16 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD11 | 4 | 0.18 | 0.06 | 0.16 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD12 | 4 | 0.18 | 0.06 | 0.16 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD13 | 4 | 0.18 | 0.06 | 0.16 |
| (1,698) | 1:106:A:ALA:HB1 | 1:124:A:GLY:HA2 | 4 | 0.18 | 0.08 | 0.14 |
| (1,698) | 1:106:A:ALA:HB2 | 1:124:A:GLY:HA2 | 4 | 0.18 | 0.08 | 0.14 |
| (1,698) | 1:106:A:ALA:HB3 | 1:124:A:GLY:HA2 | 4 | 0.18 | 0.08 | 0.14 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD11 | 4 | 0.17 | 0.05 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD12 | 4 | 0.17 | 0.05 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD13 | 4 | 0.17 | 0.05 | 0.15 |
| (1,2788) | 1:172:A:SER:H | 1:175:A:ASN:H | 4 | 0.17 | 0.03 | 0.17 |
| (1,3012) | 1:216:A:LEU:HB2 | 1:217:A:GLY:H | 4 | 0.17 | 0.02 | 0.17 |
| (1,1707) | 1:194:A:ILE:HG21 | 1:196:A:ASN:HA | 4 | 0.16 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1707) | 1:194:A:ILE:HG22 | 1:196:A:ASN:HA | 4 | 0.16 | 0.03 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG23 | 1:196:A:ASN:HA | 4 | 0.16 | 0.03 | 0.16 |
| (1,3493) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HA | 4 | 0.16 | 0.05 | 0.16 |
| (1,3493) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HA | 4 | 0.16 | 0.05 | 0.16 |
| (1,3493) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HA | 4 | 0.16 | 0.05 | 0.16 |
| (1,2605) | 1:142:A:THR:H | 1:148:A:SER:HA | 4 | 0.16 | 0.04 | 0.15 |
| (1,80) | 1:53:A:THR:HA | 2:9:B:ILE:HA | 4 | 0.16 | 0.04 | 0.14 |
| (1,79) | 1:70:A:THR:HA | 1:86:A:GLU:HB3 | 4 | 0.16 | 0.05 | 0.14 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD11 | 4 | 0.15 | 0.06 | 0.12 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD12 | 4 | 0.15 | 0.06 | 0.12 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD13 | 4 | 0.15 | 0.06 | 0.12 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD2 | 4 | 0.14 | 0.02 | 0.15 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD3 | 4 | 0.14 | 0.02 | 0.15 |
| (1,320) | 1:58:A:HIS:HB3 | 1:71:A:GLY:HA3 | 4 | 0.14 | 0.03 | 0.13 |
| (1,1567) | 1:184:A:ILE:HG21 | 1:189:A:VAL:H | 4 | 0.14 | 0.03 | 0.13 |
| (1,1567) | 1:184:A:ILE:HG22 | 1:189:A:VAL:H | 4 | 0.14 | 0.03 | 0.13 |
| (1,1567) | 1:184:A:ILE:HG23 | 1:189:A:VAL:H | 4 | 0.14 | 0.03 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG11 | 1:123:A:LYS:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG12 | 1:123:A:LYS:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG13 | 1:123:A:LYS:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG21 | 1:123:A:LYS:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG22 | 1:123:A:LYS:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG23 | 1:123:A:LYS:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,51) | 1:122:A:PRO:HD3 | 1:137:A:ASP:HB3 | 4 | 0.11 | 0.01 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB1 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB2 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB3 | 4 | 0.11 | 0.0 | 0.11 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE1 | 3 | 2.18 | 0.26 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE2 | 3 | 2.18 | 0.26 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE3 | 3 | 2.18 | 0.26 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE1 | 3 | 2.18 | 0.26 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE2 | 3 | 2.18 | 0.26 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE3 | 3 | 2.18 | 0.26 | 2.34 |
| (1,1403) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG3 | 3 | 1.98 | 0.08 | 1.95 |
| (1,1403) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG3 | 3 | 1.98 | 0.08 | 1.95 |
| (1,1411) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB2 | 3 | 1.46 | 0.09 | 1.5 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD11 | 3 | 1.41 | 0.25 | 1.42 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD12 | 3 | 1.41 | 0.25 | 1.42 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD13 | 3 | 1.41 | 0.25 | 1.42 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG2 | 3 | 1.16 | 0.62 | 1.5 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG3 | 3 | 1.16 | 0.62 | 1.5 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG2 | 3 | 1.15 | 0.85 | 1.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG3 | 3 | 1.15 | 0.85 | 1.14 |
| (1,600) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG3 | 3 | 1.1 | 0.76 | 1.22 |
| (1,600) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG3 | 3 | 1.1 | 0.76 | 1.22 |
| (1,600) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG3 | 3 | 1.1 | 0.76 | 1.22 |
| (1,1404) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG2 | 3 | 1.09 | 0.03 | 1.09 |
| (1,1404) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG2 | 3 | 1.09 | 0.03 | 1.09 |
| (1,2123) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 3 | 1.06 | 0.64 | 0.8 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG2 | 3 | 0.88 | 0.52 | 0.57 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG3 | 3 | 0.88 | 0.52 | 0.57 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG21 | 3 | 0.81 | 0.45 | 1.02 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG22 | 3 | 0.81 | 0.45 | 1.02 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG23 | 3 | 0.81 | 0.45 | 1.02 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE21 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE22 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE21 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE22 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE21 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE22 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE21 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE22 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE21 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE22 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE21 | 3 | 0.73 | 0.33 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE22 | 3 | 0.73 | 0.33 | 0.56 |
| (1,541) | 1:94:A:ALA:H | 1:97:A:GLN:HG3 | 3 | 0.73 | 0.47 | 0.6 |
| (1,1412) | 1:174:A:GLU:HG2 | 1:177:A:GLU:HB3 | 3 | 0.73 | 0.12 | 0.81 |
| (1,1413) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB3 | 3 | 0.72 | 0.13 | 0.79 |
| (1,3834) | 1:127:A:ASN:HB2 | 1:131:A:LYS:H | 3 | 0.64 | 0.29 | 0.49 |
| (1,3834) | 1:127:A:ASN:HB3 | 1:131:A:LYS:H | 3 | 0.64 | 0.29 | 0.49 |
| (1,643) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 3 | 0.63 | 0.34 | 0.74 |
| (1,1727) | 1:168:A:ALA:H | 1:196:A:ASN:HB3 | 3 | 0.59 | 0.21 | 0.49 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD21 | 3 | 0.54 | 0.28 | 0.7 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD22 | 3 | 0.54 | 0.28 | 0.7 |
| (1,2127) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB2 | 3 | 0.54 | 0.23 | 0.4 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE21 | 3 | 0.54 | 0.26 | 0.69 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE22 | 3 | 0.54 | 0.26 | 0.69 |
| (1,664) | 1:103:A:THR:HA | 1:128:A:LEU:H | 3 | 0.49 | 0.35 | 0.41 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 3 | 0.48 | 0.17 | 0.55 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 3 | 0.48 | 0.17 | 0.55 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 3 | 0.48 | 0.17 | 0.55 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 3 | 0.48 | 0.17 | 0.55 |
| (1,3530) | 1:63:A:TYR:HE1 | 2:21:B:MET:HB2 | 3 | 0.47 | 0.23 | 0.49 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3530) | 1:63:A:TYR:HE2 | 2:21:B:MET:HB2 | 3 | 0.47 | 0.23 | 0.49 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE2 | 3 | 0.44 | 0.17 | 0.52 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE3 | 3 | 0.44 | 0.17 | 0.52 |
| (1,3249) | 1:143:A:VAL:HB | 1:182:A:HIS:HE1 | 3 | 0.42 | 0.27 | 0.29 |
| (1,572) | 1:92:A:LYS:HD2 | 1:93:A:GLU:H | 3 | 0.41 | 0.18 | 0.48 |
| (1,572) | 1:92:A:LYS:HD3 | 1:93:A:GLU:H | 3 | 0.41 | 0.18 | 0.48 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 3 | 0.39 | 0.04 | 0.39 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 3 | 0.39 | 0.04 | 0.39 |
| (1,81) | 1:52:A:VAL:HG11 | 1:53:A:THR:HB | 3 | 0.38 | 0.07 | 0.38 |
| (1,81) | 1:52:A:VAL:HG12 | 1:53:A:THR:HB | 3 | 0.38 | 0.07 | 0.38 |
| (1,81) | 1:52:A:VAL:HG13 | 1:53:A:THR:HB | 3 | 0.38 | 0.07 | 0.38 |
| (1,1441) | 1:142:A:THR:HG21 | 1:178:A:ALA:HA | 3 | 0.37 | 0.18 | 0.47 |
| (1,1441) | 1:142:A:THR:HG22 | 1:178:A:ALA:HA | 3 | 0.37 | 0.18 | 0.47 |
| (1,1441) | 1:142:A:THR:HG23 | 1:178:A:ALA:HA | 3 | 0.37 | 0.18 | 0.47 |
| (1,3405) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HB3 | 3 | 0.37 | 0.31 | 0.19 |
| (1,3405) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HB3 | 3 | 0.37 | 0.31 | 0.19 |
| (1,3405) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HB3 | 3 | 0.37 | 0.31 | 0.19 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG2 | 3 | 0.36 | 0.2 | 0.3 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG3 | 3 | 0.36 | 0.2 | 0.3 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG2 | 3 | 0.36 | 0.2 | 0.3 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG3 | 3 | 0.36 | 0.2 | 0.3 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG2 | 3 | 0.36 | 0.2 | 0.3 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG3 | 3 | 0.36 | 0.2 | 0.3 |
| (1,3768) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG13 | 3 | 0.35 | 0.15 | 0.37 |
| (1,3768) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 3 | 0.35 | 0.15 | 0.37 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD2 | 3 | 0.34 | 0.14 | 0.27 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD3 | 3 | 0.34 | 0.14 | 0.27 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD2 | 3 | 0.34 | 0.14 | 0.27 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD3 | 3 | 0.34 | 0.14 | 0.27 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD2 | 3 | 0.34 | 0.14 | 0.27 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD3 | 3 | 0.34 | 0.14 | 0.27 |
| (1,261) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HZ | 3 | 0.34 | 0.17 | 0.29 |
| (1,261) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HZ | 3 | 0.34 | 0.17 | 0.29 |
| (1,261) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HZ | 3 | 0.34 | 0.17 | 0.29 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD11 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD12 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD13 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD21 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD22 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD23 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD11 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD12 | 3 | 0.33 | 0.26 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD13 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD21 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD22 | 3 | 0.33 | 0.26 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD23 | 3 | 0.33 | 0.26 | 0.16 |
| (1,37) | 1:51:A:PRO:HA | 2:7:B:PRO:HD2 | 3 | 0.32 | 0.08 | 0.37 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE1 | 3 | 0.31 | 0.2 | 0.21 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE2 | 3 | 0.31 | 0.2 | 0.21 |
| (1,3672) | 1:91:A:GLN:HB2 | 1:92:A:LYS:H | 3 | 0.3 | 0.11 | 0.35 |
| (1,3672) | 1:91:A:GLN:HB3 | 1:92:A:LYS:H | 3 | 0.3 | 0.11 | 0.35 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD11 | 3 | 0.3 | 0.16 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD12 | 3 | 0.3 | 0.16 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD13 | 3 | 0.3 | 0.16 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 3 | 0.3 | 0.16 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 3 | 0.3 | 0.16 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 3 | 0.3 | 0.16 | 0.29 |
| (1,729) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 3 | 0.29 | 0.01 | 0.28 |
| (1,2800) | 1:174:A:GLU:H | 1:174:A:GLU:HG3 | 3 | 0.28 | 0.01 | 0.28 |
| (1,3329) | 2:20:B:ARG:HD2 | 2:21:B:MET:H | 3 | 0.27 | 0.06 | 0.28 |
| (1,3329) | 2:20:B:ARG:HD3 | 2:21:B:MET:H | 3 | 0.27 | 0.06 | 0.28 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE1 | 3 | 0.27 | 0.15 | 0.23 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE2 | 3 | 0.27 | 0.15 | 0.23 |
| (1,3126) | 1:112:A:TYR:HE1 | 1:114:A:ASP:H | 3 | 0.27 | 0.11 | 0.27 |
| (1,3126) | 1:112:A:TYR:HE2 | 1:114:A:ASP:H | 3 | 0.27 | 0.11 | 0.27 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 3 | 0.27 | 0.01 | 0.27 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 3 | 0.27 | 0.01 | 0.27 |
| (1,1380) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB2 | 3 | 0.27 | 0.05 | 0.29 |
| (1,1380) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB2 | 3 | 0.27 | 0.05 | 0.29 |
| (1,1380) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB2 | 3 | 0.27 | 0.05 | 0.29 |
| (1,3643) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 3 | 0.26 | 0.01 | 0.26 |
| (1,3643) | 1:85:A:ASP:HB3 | 1:108:A:GLY:HA2 | 3 | 0.26 | 0.01 | 0.26 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD2 | 3 | 0.26 | 0.06 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD3 | 3 | 0.26 | 0.06 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD2 | 3 | 0.26 | 0.06 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD3 | 3 | 0.26 | 0.06 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD2 | 3 | 0.26 | 0.06 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD3 | 3 | 0.26 | 0.06 | 0.25 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB2 | 3 | 0.25 | 0.07 | 0.28 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 3 | 0.25 | 0.07 | 0.28 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB2 | 3 | 0.25 | 0.07 | 0.28 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 3 | 0.25 | 0.07 | 0.28 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB2 | 3 | 0.25 | 0.07 | 0.28 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 3 | 0.25 | 0.07 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB1 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB2 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB3 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB1 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB2 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB3 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB1 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB2 | 3 | 0.25 | 0.1 | 0.2 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB3 | 3 | 0.25 | 0.1 | 0.2 |
| (1,3096) | 1:60:A:LYS:HE3 | 1:61:A:GLY:H | 3 | 0.25 | 0.12 | 0.22 |
| (1,1363) | 1:153:A:VAL:H | 1:166:A:ASP:HB2 | 3 | 0.23 | 0.02 | 0.23 |
| (1,462) | 1:81:A:ARG:HA | 1:81:A:ARG:HD3 | 3 | 0.22 | 0.02 | 0.21 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD11 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD12 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD13 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD11 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD12 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD13 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD11 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD12 | 3 | 0.22 | 0.09 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD13 | 3 | 0.22 | 0.09 | 0.19 |
| (1,170) | 1:56:A:ALA:HB1 | 1:69:A:PHE:H | 3 | 0.22 | 0.06 | 0.26 |
| (1,170) | 1:56:A:ALA:HB2 | 1:69:A:PHE:H | 3 | 0.22 | 0.06 | 0.26 |
| (1,170) | 1:56:A:ALA:HB3 | 1:69:A:PHE:H | 3 | 0.22 | 0.06 | 0.26 |
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG2 | 3 | 0.21 | 0.1 | 0.15 |
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG3 | 3 | 0.21 | 0.1 | 0.15 |
| (1,1997) | 1:184:A:ILE:HA | 1:216:A:LEU:HB3 | 3 | 0.21 | 0.06 | 0.21 |
| (1,2652) | 1:149:A:ALA:H | 1:179:A:LEU:HB3 | 3 | 0.21 | 0.07 | 0.2 |
| (1,143) | 1:53:A:THR:HG21 | 1:55:A:ASN:HB3 | 3 | 0.2 | 0.09 | 0.14 |
| (1,143) | 1:53:A:THR:HG22 | 1:55:A:ASN:HB3 | 3 | 0.2 | 0.09 | 0.14 |
| (1,143) | 1:53:A:THR:HG23 | 1:55:A:ASN:HB3 | 3 | 0.2 | 0.09 | 0.14 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG21 | 3 | 0.2 | 0.07 | 0.21 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG22 | 3 | 0.2 | 0.07 | 0.21 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG23 | 3 | 0.2 | 0.07 | 0.21 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB2 | 3 | 0.2 | 0.05 | 0.22 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB3 | 3 | 0.2 | 0.05 | 0.22 |
| (1,1053) | 1:139:A:SER:HB3 | 1:140:A:ILE:H | 3 | 0.2 | 0.05 | 0.21 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB2 | 3 | 0.2 | 0.08 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB3 | 3 | 0.2 | 0.08 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB2 | 3 | 0.2 | 0.08 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB3 | 3 | 0.2 | 0.08 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB2 | 3 | 0.2 | 0.08 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB3 | 3 | 0.2 | 0.08 | 0.2 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB1 | 3 | 0.19 | 0.12 | 0.11 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB2 | 3 | 0.19 | 0.12 | 0.11 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB3 | 3 | 0.19 | 0.12 | 0.11 |
| (1,2393) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 3 | 0.19 | 0.06 | 0.18 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG11 | 3 | 0.19 | 0.02 | 0.2 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG12 | 3 | 0.19 | 0.02 | 0.2 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG13 | 3 | 0.19 | 0.02 | 0.2 |
| (1,2927) | 1:195:A:ASN:HB2 | 1:196:A:ASN:H | 3 | 0.19 | 0.05 | 0.2 |
| (1,526) | 1:87:A:VAL:HG11 | 1:104:A:VAL:HA | 3 | 0.19 | 0.06 | 0.21 |
| (1,526) | 1:87:A:VAL:HG12 | 1:104:A:VAL:HA | 3 | 0.19 | 0.06 | 0.21 |
| (1,526) | 1:87:A:VAL:HG13 | 1:104:A:VAL:HA | 3 | 0.19 | 0.06 | 0.21 |
| (1,526) | 1:87:A:VAL:HG21 | 1:104:A:VAL:HA | 3 | 0.19 | 0.06 | 0.21 |
| (1,526) | 1:87:A:VAL:HG22 | 1:104:A:VAL:HA | 3 | 0.19 | 0.06 | 0.21 |
| (1,526) | 1:87:A:VAL:HG23 | 1:104:A:VAL:HA | 3 | 0.19 | 0.06 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD2 | 3 | 0.19 | 0.04 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD3 | 3 | 0.19 | 0.04 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 3 | 0.19 | 0.04 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 3 | 0.19 | 0.04 | 0.21 |
| (1,409) | 1:75:A:ILE:HG21 | 1:76:A:MET:HA | 3 | 0.18 | 0.05 | 0.16 |
| (1,409) | 1:75:A:ILE:HG22 | 1:76:A:MET:HA | 3 | 0.18 | 0.05 | 0.16 |
| (1,409) | 1:75:A:ILE:HG23 | 1:76:A:MET:HA | 3 | 0.18 | 0.05 | 0.16 |
| (1,655) | 1:102:A:ARG:HD2 | 1:103:A:THR:H | 3 | 0.17 | 0.1 | 0.11 |
| (1,655) | 1:102:A:ARG:HD3 | 1:103:A:THR:H | 3 | 0.17 | 0.1 | 0.11 |
| (1,1815) | 1:201:A:ILE:HG21 | 1:205:A:LYS:H | 3 | 0.17 | 0.07 | 0.14 |
| (1,1815) | 1:201:A:ILE:HG22 | 1:205:A:LYS:H | 3 | 0.17 | 0.07 | 0.14 |
| (1,1815) | 1:201:A:ILE:HG23 | 1:205:A:LYS:H | 3 | 0.17 | 0.07 | 0.14 |
| (1,2950) | 1:198:A:THR:HA | 1:199:A:GLY:H | 3 | 0.17 | 0.05 | 0.19 |
| (1,1006) | 1:136:A:TYR:HB3 | 1:152:A:LYS:HA | 3 | 0.17 | 0.05 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD11 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD12 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD13 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD21 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD22 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD23 | 3 | 0.16 | 0.03 | 0.15 |
| (1,990) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HB | 3 | 0.16 | 0.03 | 0.17 |
| (1,1542) | 1:184:A:ILE:HA | 1:189:A:VAL:HB | 3 | 0.16 | 0.03 | 0.16 |
| (1,3462) | 2:17:B:LYS:HA | 2:17:B:LYS:HG2 | 3 | 0.15 | 0.01 | 0.15 |
| (1,317) | 1:218:A:ALA:HB1 | 1:220:A:LEU:HA | 3 | 0.15 | 0.05 | 0.12 |
| (1,317) | 1:218:A:ALA:HB2 | 1:220:A:LEU:HA | 3 | 0.15 | 0.05 | 0.12 |
| (1,317) | 1:218:A:ALA:HB3 | 1:220:A:LEU:HA | 3 | 0.15 | 0.05 | 0.12 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG11 | 3 | 0.15 | 0.04 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG12 | 3 | 0.15 | 0.04 | 0.15 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG13 | 3 | 0.15 | 0.04 | 0.15 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG21 | 3 | 0.14 | 0.01 | 0.14 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG22 | 3 | 0.14 | 0.01 | 0.14 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG23 | 3 | 0.14 | 0.01 | 0.14 |
| (1,1360) | 1:153:A:VAL:HB | 1:166:A:ASP:HB2 | 3 | 0.14 | 0.02 | 0.13 |
| (1,1549) | 1:184:A:ILE:HD11 | 1:219:A:THR:H | 3 | 0.14 | 0.02 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD12 | 1:219:A:THR:H | 3 | 0.14 | 0.02 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD13 | 1:219:A:THR:H | 3 | 0.14 | 0.02 | 0.12 |
| (1,950) | 1:130:A:THR:HB | 1:131:A:LYS:H | 3 | 0.14 | 0.03 | 0.12 |
| (1,1674) | 1:192:A:ILE:HG21 | 1:193:A:THR:HB | 3 | 0.14 | 0.03 | 0.12 |
| (1,1674) | 1:192:A:ILE:HG22 | 1:193:A:THR:HB | 3 | 0.14 | 0.03 | 0.12 |
| (1,1674) | 1:192:A:ILE:HG23 | 1:193:A:THR:HB | 3 | 0.14 | 0.03 | 0.12 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB2 | 3 | 0.14 | 0.03 | 0.12 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB3 | 3 | 0.14 | 0.03 | 0.12 |
| (1,353) | 1:73:A:VAL:HG11 | 1:74:A:ASP:HA | 3 | 0.13 | 0.03 | 0.13 |
| (1,353) | 1:73:A:VAL:HG12 | 1:74:A:ASP:HA | 3 | 0.13 | 0.03 | 0.13 |
| (1,353) | 1:73:A:VAL:HG13 | 1:74:A:ASP:HA | 3 | 0.13 | 0.03 | 0.13 |
| (1,2294) | 1:76:A:MET:HB3 | 1:77:A:GLN:H | 3 | 0.13 | 0.01 | 0.14 |
| (1,1545) | 1:184:A:ILE:HA | 1:189:A:VAL:HA | 3 | 0.13 | 0.01 | 0.14 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD11 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD12 | 3 | 0.13 | 0.01 | 0.13 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD13 | 3 | 0.13 | 0.01 | 0.13 |
| (1,444) | 1:77:A:GLN:HA | 1:78:A:GLY:HA3 | 3 | 0.12 | 0.01 | 0.13 |
| (1,3264) | 1:58:A:HIS:HD2 | 1:60:A:LYS:H | 3 | 0.12 | 0.02 | 0.11 |
| (1,35) | 1:155:A:LYS:HB3 | 1:155:A:LYS:HE2 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1204) | 1:152:A:LYS:H | 1:152:A:LYS:HG3 | 3 | 0.12 | 0.01 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG11 | 1:102:A:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG12 | 1:102:A:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG13 | 1:102:A:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG21 | 1:102:A:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG22 | 1:102:A:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG23 | 1:102:A:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,1691) | 1:194:A:ILE:HD11 | 1:223:A:THR:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,1691) | 1:194:A:ILE:HD12 | 1:223:A:THR:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,1691) | 1:194:A:ILE:HD13 | 1:223:A:THR:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD21 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD22 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD23 | 3 | 0.11 | 0.0 | 0.11 |
| (1,338) | 1:172:A:SER:HA | 1:173:A:TYR:HA | 3 | 0.11 | 0.01 | 0.11 |
| (1,3272) | 1:111:A:HIS:HB3 | 1:111:A:HIS:HD2 | 3 | 0.11 | 0.01 | 0.11 |
| (1,2314) | 1:83:A:GLN:H | 1:83:A:GLN:HB3 | 3 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,897) | 1:123:A:LYS:HE2 | 1:136:A:TYR:HB3 | 2 | 1.68 | 0.63 | 1.68 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD21 | 2 | 1.2 | 0.33 | 1.2 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD22 | 2 | 1.2 | 0.33 | 1.2 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD23 | 2 | 1.2 | 0.33 | 1.2 |
| (1,14) | 1:47:A:THR:HB | 1:49:A:ASP:H | 2 | 1.04 | 0.15 | 1.04 |
| (1,3623) | 1:81:A:ARG:HD2 | 1:83:A:GLN:HG2 | 2 | 0.98 | 0.14 | 0.98 |
| (1,3623) | 1:81:A:ARG:HD3 | 1:83:A:GLN:HG2 | 2 | 0.98 | 0.14 | 0.98 |
| (1,896) | 1:123:A:LYS:HE3 | 1:136:A:TYR:HB3 | 2 | 0.96 | 0.21 | 0.96 |
| (1,2229) | 1:66:A:ASP:H | 1:67:A:ALA:H | 2 | 0.88 | 0.19 | 0.88 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD11 | 2 | 0.85 | 0.42 | 0.85 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD12 | 2 | 0.85 | 0.42 | 0.85 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD13 | 2 | 0.85 | 0.42 | 0.85 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD21 | 2 | 0.85 | 0.42 | 0.85 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD22 | 2 | 0.85 | 0.42 | 0.85 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD23 | 2 | 0.85 | 0.42 | 0.85 |
| (1,4019) | 2:12:B:ASN:HD22 | 2:13:B:ARG:HB2 | 2 | 0.85 | 0.36 | 0.85 |
| (1,4019) | 2:12:B:ASN:HD22 | 2:13:B:ARG:HB3 | 2 | 0.85 | 0.36 | 0.85 |
| (1,580) | 1:91:A:GLN:HA | 1:92:A:LYS:HG2 | 2 | 0.76 | 0.02 | 0.76 |
| (1,580) | 1:91:A:GLN:HA | 1:92:A:LYS:HG3 | 2 | 0.76 | 0.02 | 0.76 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG11 | 2 | 0.75 | 0.16 | 0.75 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG12 | 2 | 0.75 | 0.16 | 0.75 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG13 | 2 | 0.75 | 0.16 | 0.75 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG11 | 2 | 0.75 | 0.16 | 0.75 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG12 | 2 | 0.75 | 0.16 | 0.75 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG13 | 2 | 0.75 | 0.16 | 0.75 |
| (1,3406) | 2:8:B:ILE:HD11 | 2:21:B:MET:HG3 | 2 | 0.74 | 0.44 | 0.74 |
| (1,3406) | 2:8:B:ILE:HD12 | 2:21:B:MET:HG3 | 2 | 0.74 | 0.44 | 0.74 |
| (1,3406) | 2:8:B:ILE:HD13 | 2:21:B:MET:HG3 | 2 | 0.74 | 0.44 | 0.74 |
| (1,782) | 1:80:A:SER:HB2 | 1:114:A:ASP:HB3 | 2 | 0.72 | 0.14 | 0.72 |
| (1,3843) | 1:137:A:ASP:H | 1:152:A:LYS:HE2 | 2 | 0.71 | 0.15 | 0.71 |
| (1,3843) | 1:137:A:ASP:H | 1:152:A:LYS:HE3 | 2 | 0.71 | 0.15 | 0.71 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG21 | 2 | 0.66 | 0.24 | 0.66 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG22 | 2 | 0.66 | 0.24 | 0.66 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG23 | 2 | 0.66 | 0.24 | 0.66 |
| (1,3206) | 1:88:A:GLN:HG2 | 1:90:A:HIS:HE1 | 2 | 0.66 | 0.11 | 0.66 |
| (1,3123) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HE1 | 2 | 0.66 | 0.55 | 0.66 |
| (1,3123) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HE2 | 2 | 0.66 | 0.55 | 0.66 |
| (1,3123) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HE1 | 2 | 0.66 | 0.55 | 0.66 |
| (1,3123) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HE2 | 2 | 0.66 | 0.55 | 0.66 |
| (1,3123) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HE1 | 2 | 0.66 | 0.55 | 0.66 |
| (1,3123) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HE2 | 2 | 0.66 | 0.55 | 0.66 |
| (1,3683) | 1:94:A:ALA:H | 1:97:A:GLN:HB2 | 2 | 0.64 | 0.08 | 0.64 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3683) | 1:94:A:ALA:H | 1:97:A:GLN:HB3 | 2 | 0.64 | 0.08 | 0.64 |
| (1,3437) | 2:12:B:ASN:HB2 | 2:16:B:GLY:H | 2 | 0.62 | 0.5 | 0.62 |
| (1,3055) | 1:193:A:THR:HG21 | 1:195:A:ASN:HD21 | 2 | 0.62 | 0.04 | 0.62 |
| (1,3055) | 1:193:A:THR:HG22 | 1:195:A:ASN:HD21 | 2 | 0.62 | 0.04 | 0.62 |
| (1,3055) | 1:193:A:THR:HG23 | 1:195:A:ASN:HD21 | 2 | 0.62 | 0.04 | 0.62 |
| (1,2139) | 1:48:A:ASN:H | 1:49:A:ASP:H | 2 | 0.59 | 0.03 | 0.59 |
| (1,3387) | 2:8:B:ILE:HD11 | 2:21:B:MET:H | 2 | 0.56 | 0.31 | 0.56 |
| (1,3387) | 2:8:B:ILE:HD12 | 2:21:B:MET:H | 2 | 0.56 | 0.31 | 0.56 |
| (1,3387) | 2:8:B:ILE:HD13 | 2:21:B:MET:H | 2 | 0.56 | 0.31 | 0.56 |
| (1,3159) | 1:112:A:TYR:HD1 | 1:135:A:PHE:HD1 | 2 | 0.55 | 0.01 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD1 | 1:135:A:PHE:HD2 | 2 | 0.55 | 0.01 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD2 | 1:135:A:PHE:HD1 | 2 | 0.55 | 0.01 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD2 | 1:135:A:PHE:HD2 | 2 | 0.55 | 0.01 | 0.55 |
| (1,1057) | 1:139:A:SER:HB3 | 1:151:A:ALA:H | 2 | 0.54 | 0.29 | 0.54 |
| (1,2645) | 1:148:A:SER:H | 1:179:A:LEU:HB3 | 2 | 0.52 | 0.35 | 0.52 |
| (1,3104) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HD1 | 2 | 0.51 | 0.33 | 0.51 |
| (1,3104) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HD2 | 2 | 0.51 | 0.33 | 0.51 |
| (1,386) | 1:75:A:ILE:HD11 | 1:84:A:ALA:H | 2 | 0.5 | 0.05 | 0.5 |
| (1,386) | 1:75:A:ILE:HD12 | 1:84:A:ALA:H | 2 | 0.5 | 0.05 | 0.5 |
| (1,386) | 1:75:A:ILE:HD13 | 1:84:A:ALA:H | 2 | 0.5 | 0.05 | 0.5 |
| (1,3547) | 1:52:A:VAL:HG11 | 1:77:A:GLN:HG2 | 2 | 0.5 | 0.1 | 0.5 |
| (1,3547) | 1:52:A:VAL:HG11 | 1:77:A:GLN:HG3 | 2 | 0.5 | 0.1 | 0.5 |
| (1,3547) | 1:52:A:VAL:HG12 | 1:77:A:GLN:HG2 | 2 | 0.5 | 0.1 | 0.5 |
| (1,3547) | 1:52:A:VAL:HG12 | 1:77:A:GLN:HG3 | 2 | 0.5 | 0.1 | 0.5 |
| (1,3547) | 1:52:A:VAL:HG13 | 1:77:A:GLN:HG2 | 2 | 0.5 | 0.1 | 0.5 |
| (1,3547) | 1:52:A:VAL:HG13 | 1:77:A:GLN:HG3 | 2 | 0.5 | 0.1 | 0.5 |
| (1,3401) | 2:6:B:VAL:HG21 | 2:7:B:PRO:HD3 | 2 | 0.5 | 0.13 | 0.5 |
| (1,3401) | 2:6:B:VAL:HG22 | 2:7:B:PRO:HD3 | 2 | 0.5 | 0.13 | 0.5 |
| (1,3401) | 2:6:B:VAL:HG23 | 2:7:B:PRO:HD3 | 2 | 0.5 | 0.13 | 0.5 |
| (1,2638) | 1:142:A:THR:HG21 | 1:147:A:GLY:H | 2 | 0.5 | 0.18 | 0.5 |
| (1,2638) | 1:142:A:THR:HG22 | 1:147:A:GLY:H | 2 | 0.5 | 0.18 | 0.5 |
| (1,2638) | 1:142:A:THR:HG23 | 1:147:A:GLY:H | 2 | 0.5 | 0.18 | 0.5 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD11 | 2 | 0.48 | 0.12 | 0.48 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD12 | 2 | 0.48 | 0.12 | 0.48 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD13 | 2 | 0.48 | 0.12 | 0.48 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD21 | 2 | 0.48 | 0.12 | 0.48 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD22 | 2 | 0.48 | 0.12 | 0.48 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD23 | 2 | 0.48 | 0.12 | 0.48 |
| (1,475) | 1:82:A:LEU:HA | 1:112:A:TYR:HD1 | 2 | 0.47 | 0.13 | 0.47 |
| (1,475) | 1:82:A:LEU:HA | 1:112:A:TYR:HD2 | 2 | 0.47 | 0.13 | 0.47 |
| (1,3949) | 1:193:A:THR:HB | 1:195:A:ASN:HD21 | 2 | 0.46 | 0.02 | 0.46 |
| (1,3949) | 1:193:A:THR:HB | 1:195:A:ASN:HD22 | 2 | 0.46 | 0.02 | 0.46 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,780) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG12 | 2 | 0.46 | 0.22 | 0.46 |
| (1,68) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG2 | 2 | 0.45 | 0.01 | 0.45 |
| (1,68) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG2 | 2 | 0.45 | 0.01 | 0.45 |
| (1,68) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG2 | 2 | 0.45 | 0.01 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HG2 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HG3 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HG2 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HG3 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HG2 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HG3 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HG2 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HG3 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HG2 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HG3 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HG2 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3663) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HG3 | 2 | 0.45 | 0.23 | 0.45 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG21 | 2 | 0.44 | 0.1 | 0.44 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG22 | 2 | 0.44 | 0.1 | 0.44 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG23 | 2 | 0.44 | 0.1 | 0.44 |
| (1,414) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HA | 2 | 0.44 | 0.04 | 0.44 |
| (1,414) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HA | 2 | 0.44 | 0.04 | 0.44 |
| (1,414) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HA | 2 | 0.44 | 0.04 | 0.44 |
| (1,2141) | 1:49:A:ASP:HA | 1:50:A:LEU:H | 2 | 0.44 | 0.1 | 0.44 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG21 | 2 | 0.44 | 0.33 | 0.44 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG22 | 2 | 0.44 | 0.33 | 0.44 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG23 | 2 | 0.44 | 0.33 | 0.44 |
| (1,3429) | 2:4:B:LYS:HA | 2:4:B:LYS:HD2 | 2 | 0.44 | 0.02 | 0.44 |
| (1,3429) | 2:4:B:LYS:HA | 2:4:B:LYS:HD3 | 2 | 0.44 | 0.02 | 0.44 |
| (1,3508) | 1:51:A:PRO:HB2 | 2:7:B:PRO:HD2 | 2 | 0.41 | 0.09 | 0.41 |
| (1,3703) | 1:102:A:ARG:H | 1:129:A:ASN:HD21 | 2 | 0.41 | 0.29 | 0.41 |
| (1,3703) | 1:102:A:ARG:H | 1:129:A:ASN:HD22 | 2 | 0.41 | 0.29 | 0.41 |
| (1,3067) | 1:167:A:ASP:HA | 1:196:A:ASN:HD21 | 2 | 0.39 | 0.14 | 0.39 |
| (1,69) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE21 | 2 | 0.36 | 0.24 | 0.36 |
| (1,69) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE21 | 2 | 0.36 | 0.24 | 0.36 |
| (1,69) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE21 | 2 | 0.36 | 0.24 | 0.36 |
| (1,196) | 1:167:A:ASP:HA | 1:196:A:ASN:HB2 | 2 | 0.36 | 0.1 | 0.36 |
| (1,2190) | 1:58:A:HIS:H | 2:12:B:ASN:HD22 | 2 | 0.35 | 0.15 | 0.35 |
| (1,794) | 1:73:A:VAL:HG11 | 1:83:A:GLN:HG2 | 2 | 0.34 | 0.06 | 0.34 |
| (1,794) | 1:73:A:VAL:HG12 | 1:83:A:GLN:HG2 | 2 | 0.34 | 0.06 | 0.34 |
| (1,794) | 1:73:A:VAL:HG13 | 1:83:A:GLN:HG2 | 2 | 0.34 | 0.06 | 0.34 |
| (1,1050) | 1:139:A:SER:HB3 | 1:150:A:SER:HA | 2 | 0.34 | 0.16 | 0.34 |
| (1,2376) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 2 | 0.34 | 0.01 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3281) | 1:54:A:ILE:HD11 | 1:69:A:PHE:HZ | 2 | 0.34 | 0.2 | 0.34 |
| (1,3281) | 1:54:A:ILE:HD12 | 1:69:A:PHE:HZ | 2 | 0.34 | 0.2 | 0.34 |
| (1,3281) | 1:54:A:ILE:HD13 | 1:69:A:PHE:HZ | 2 | 0.34 | 0.2 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD11 | 1:221:A:THR:HA | 2 | 0.32 | 0.02 | 0.32 |
| (1,3991) | 1:220:A:LEU:HD12 | 1:221:A:THR:HA | 2 | 0.32 | 0.02 | 0.32 |
| (1,3991) | 1:220:A:LEU:HD13 | 1:221:A:THR:HA | 2 | 0.32 | 0.02 | 0.32 |
| (1,3991) | 1:220:A:LEU:HD21 | 1:221:A:THR:HA | 2 | 0.32 | 0.02 | 0.32 |
| (1,3991) | 1:220:A:LEU:HD22 | 1:221:A:THR:HA | 2 | 0.32 | 0.02 | 0.32 |
| (1,3991) | 1:220:A:LEU:HD23 | 1:221:A:THR:HA | 2 | 0.32 | 0.02 | 0.32 |
| (1,1120) | 1:142:A:THR:HG21 | 1:179:A:LEU:H | 2 | 0.31 | 0.05 | 0.31 |
| (1,1120) | 1:142:A:THR:HG22 | 1:179:A:LEU:H | 2 | 0.31 | 0.05 | 0.31 |
| (1,1120) | 1:142:A:THR:HG23 | 1:179:A:LEU:H | 2 | 0.31 | 0.05 | 0.31 |
| (1,1284) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 2 | 0.31 | 0.04 | 0.31 |
| (1,1284) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 2 | 0.31 | 0.04 | 0.31 |
| (1,1284) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 2 | 0.31 | 0.04 | 0.31 |
| (1,4046) | 2:19:B:GLN:HG2 | 2:21:B:MET:H | 2 | 0.31 | 0.06 | 0.31 |
| (1,4046) | 2:19:B:GLN:HG3 | 2:21:B:MET:H | 2 | 0.31 | 0.06 | 0.31 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG21 | 2 | 0.3 | 0.18 | 0.3 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG22 | 2 | 0.3 | 0.18 | 0.3 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG23 | 2 | 0.3 | 0.18 | 0.3 |
| (1,3172) | 1:140:A:ILE:HB | 1:165:A:PHE:HZ | 2 | 0.3 | 0.1 | 0.3 |
| (1,3068) | 1:195:A:ASN:HA | 1:196:A:ASN:HD21 | 2 | 0.3 | 0.01 | 0.3 |
| (1,3223) | 1:103:A:THR:HB | 1:125:A:TRP:HD1 | 2 | 0.3 | 0.05 | 0.3 |
| (1,1161) | 1:147:A:GLY:HA2 | 1:148:A:SER:HB2 | 2 | 0.29 | 0.16 | 0.29 |
| (1,1161) | 1:147:A:GLY:HA2 | 1:148:A:SER:HB3 | 2 | 0.29 | 0.16 | 0.29 |
| (1,938) | 1:103:A:THR:HA | 1:128:A:LEU:HG | 2 | 0.29 | 0.16 | 0.29 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG21 | 2 | 0.28 | 0.08 | 0.28 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG22 | 2 | 0.28 | 0.08 | 0.28 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG23 | 2 | 0.28 | 0.08 | 0.28 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG21 | 2 | 0.28 | 0.08 | 0.28 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG22 | 2 | 0.28 | 0.08 | 0.28 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG23 | 2 | 0.28 | 0.08 | 0.28 |
| (1,1127) | 1:117:A:VAL:HA | 1:143:A:VAL:HA | 2 | 0.28 | 0.17 | 0.28 |
| (1,2016) | 1:190:A:LYS:HG3 | 1:218:A:ALA:HA | 2 | 0.28 | 0.02 | 0.28 |
| (1,3654) | 1:88:A:GLN:HG2 | 1:90:A:HIS:HE1 | 2 | 0.28 | 0.14 | 0.28 |
| (1,3654) | 1:88:A:GLN:HG3 | 1:90:A:HIS:HE1 | 2 | 0.28 | 0.14 | 0.28 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB1 | 2 | 0.28 | 0.1 | 0.28 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB2 | 2 | 0.28 | 0.1 | 0.28 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB3 | 2 | 0.28 | 0.1 | 0.28 |
| (1,425) | 1:53:A:THR:HG21 | 1:76:A:MET:HG2 | 2 | 0.26 | 0.06 | 0.26 |
| (1,425) | 1:53:A:THR:HG21 | 1:76:A:MET:HG3 | 2 | 0.26 | 0.06 | 0.26 |
| (1,425) | 1:53:A:THR:HG22 | 1:76:A:MET:HG2 | 2 | 0.26 | 0.06 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,425) | 1:53:A:THR:HG22 | 1:76:A:MET:HG3 | 2 | 0.26 | 0.06 | 0.26 |
| (1,425) | 1:53:A:THR:HG23 | 1:76:A:MET:HG2 | 2 | 0.26 | 0.06 | 0.26 |
| (1,425) | 1:53:A:THR:HG23 | 1:76:A:MET:HG3 | 2 | 0.26 | 0.06 | 0.26 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG21 | 2 | 0.26 | 0.02 | 0.26 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG22 | 2 | 0.26 | 0.02 | 0.26 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG23 | 2 | 0.26 | 0.02 | 0.26 |
| (1,1305) | 1:161:A:LYS:HD2 | 1:189:A:VAL:HA | 2 | 0.26 | 0.12 | 0.26 |
| (1,1305) | 1:161:A:LYS:HD3 | 1:189:A:VAL:HA | 2 | 0.26 | 0.12 | 0.26 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB1 | 2 | 0.26 | 0.08 | 0.26 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB2 | 2 | 0.26 | 0.08 | 0.26 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB3 | 2 | 0.26 | 0.08 | 0.26 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB1 | 2 | 0.26 | 0.08 | 0.26 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB2 | 2 | 0.26 | 0.08 | 0.26 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB3 | 2 | 0.26 | 0.08 | 0.26 |
| (1,675) | 1:103:A:THR:HG21 | 1:125:A:TRP:HZ2 | 2 | 0.25 | 0.0 | 0.25 |
| (1,675) | 1:103:A:THR:HG22 | 1:125:A:TRP:HZ2 | 2 | 0.25 | 0.0 | 0.25 |
| (1,675) | 1:103:A:THR:HG23 | 1:125:A:TRP:HZ2 | 2 | 0.25 | 0.0 | 0.25 |
| (1,3160) | 1:133:A:TRP:HH2 | 1:135:A:PHE:HD1 | 2 | 0.24 | 0.08 | 0.24 |
| (1,3160) | 1:133:A:TRP:HH2 | 1:135:A:PHE:HD2 | 2 | 0.24 | 0.08 | 0.24 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 2 | 0.23 | 0.06 | 0.23 |
| (1,105) | 1:54:A:ILE:HB | 2:9:B:ILE:H | 2 | 0.22 | 0.03 | 0.22 |
| (1,538) | 1:68:A:VAL:HG11 | 1:88:A:GLN:HG3 | 2 | 0.22 | 0.0 | 0.22 |
| (1,538) | 1:68:A:VAL:HG12 | 1:88:A:GLN:HG3 | 2 | 0.22 | 0.0 | 0.22 |
| (1,538) | 1:68:A:VAL:HG13 | 1:88:A:GLN:HG3 | 2 | 0.22 | 0.0 | 0.22 |
| (1,538) | 1:68:A:VAL:HG21 | 1:88:A:GLN:HG3 | 2 | 0.22 | 0.0 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,538) | 1:68:A:VAL:HG22 | 1:88:A:GLN:HG3 | 2 | 0.22 | 0.0 | 0.22 |
| (1,538) | 1:68:A:VAL:HG23 | 1:88:A:GLN:HG3 | 2 | 0.22 | 0.0 | 0.22 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD11 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD12 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD13 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD21 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD22 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD23 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD11 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD12 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD13 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD21 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD22 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD23 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD11 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD12 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD13 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD21 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD22 | 2 | 0.22 | 0.03 | 0.22 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD23 | 2 | 0.22 | 0.03 | 0.22 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB1 | 2 | 0.22 | 0.01 | 0.22 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB2 | 2 | 0.22 | 0.01 | 0.22 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB3 | 2 | 0.22 | 0.01 | 0.22 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB1 | 2 | 0.22 | 0.01 | 0.22 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB2 | 2 | 0.22 | 0.01 | 0.22 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB3 | 2 | 0.22 | 0.01 | 0.22 |
| (1,63) | 1:52:A:VAL:HG11 | 2:8:B:ILE:HA | 2 | 0.22 | 0.04 | 0.22 |
| (1,63) | 1:52:A:VAL:HG12 | 2:8:B:ILE:HA | 2 | 0.22 | 0.04 | 0.22 |
| (1,63) | 1:52:A:VAL:HG13 | 2:8:B:ILE:HA | 2 | 0.22 | 0.04 | 0.22 |
| (1,83) | 1:53:A:THR:HB | 1:76:A:MET:HB3 | 2 | 0.22 | 0.04 | 0.22 |
| (1,101) | 1:53:A:THR:HG21 | 1:55:A:ASN:HD21 | 2 | 0.22 | 0.02 | 0.22 |
| (1,101) | 1:53:A:THR:HG22 | 1:55:A:ASN:HD21 | 2 | 0.22 | 0.02 | 0.22 |
| (1,101) | 1:53:A:THR:HG23 | 1:55:A:ASN:HD21 | 2 | 0.22 | 0.02 | 0.22 |
| (1,1220) | 1:53:A:THR:HG21 | 1:55:A:ASN:H | 2 | 0.22 | 0.04 | 0.22 |
| (1,1220) | 1:53:A:THR:HG22 | 1:55:A:ASN:H | 2 | 0.22 | 0.04 | 0.22 |
| (1,1220) | 1:53:A:THR:HG23 | 1:55:A:ASN:H | 2 | 0.22 | 0.04 | 0.22 |
| (1,2372) | 1:92:A:LYS:H | 1:92:A:LYS:HG2 | 2 | 0.21 | 0.03 | 0.21 |
| (1,2372) | 1:92:A:LYS:H | 1:92:A:LYS:HG3 | 2 | 0.21 | 0.03 | 0.21 |
| (1,537) | 1:68:A:VAL:HG11 | 1:88:A:GLN:HG2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,537) | 1:68:A:VAL:HG12 | 1:88:A:GLN:HG2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,537) | 1:68:A:VAL:HG13 | 1:88:A:GLN:HG2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,537) | 1:68:A:VAL:HG21 | 1:88:A:GLN:HG2 | 2 | 0.2 | 0.06 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,537) | 1:68:A:VAL:HG22 | 1:88:A:GLN:HG2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,537) | 1:68:A:VAL:HG23 | 1:88:A:GLN:HG2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG21 | 2 | 0.2 | 0.08 | 0.2 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG22 | 2 | 0.2 | 0.08 | 0.2 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG23 | 2 | 0.2 | 0.08 | 0.2 |
| (1,2381) | 1:98:A:PRO:HG2 | 1:99:A:GLU:H | 2 | 0.2 | 0.02 | 0.2 |
| (1,2381) | 1:98:A:PRO:HG3 | 1:99:A:GLU:H | 2 | 0.2 | 0.02 | 0.2 |
| (1,2543) | 1:130:A:THR:HG21 | 1:131:A:LYS:H | 2 | 0.2 | 0.09 | 0.2 |
| (1,2543) | 1:130:A:THR:HG22 | 1:131:A:LYS:H | 2 | 0.2 | 0.09 | 0.2 |
| (1,2543) | 1:130:A:THR:HG23 | 1:131:A:LYS:H | 2 | 0.2 | 0.09 | 0.2 |
| (1,3716) | 1:105:A:ASP:HB2 | 1:125:A:TRP:HA | 2 | 0.2 | 0.02 | 0.2 |
| (1,3716) | 1:105:A:ASP:HB3 | 1:125:A:TRP:HA | 2 | 0.2 | 0.02 | 0.2 |
| (1,513) | 1:123:A:LYS:HB3 | 1:123:A:LYS:HD3 | 2 | 0.19 | 0.04 | 0.19 |
| (1,976) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HB3 | 2 | 0.19 | 0.01 | 0.19 |
| (1,976) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HB3 | 2 | 0.19 | 0.01 | 0.19 |
| (1,976) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HB3 | 2 | 0.19 | 0.01 | 0.19 |
| (1,2211) | 1:60:A:LYS:H | 1:60:A:LYS:HE3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3352) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3352) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,1722) | 1:195:A:ASN:HB3 | 1:196:A:ASN:HA | 2 | 0.18 | 0.05 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB1 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB2 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB3 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB1 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB2 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB3 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB1 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB2 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB3 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1397) | 1:174:A:GLU:HA | 1:177:A:GLU:HA | 2 | 0.18 | 0.03 | 0.18 |
| (1,2754) | 1:153:A:VAL:HB | 1:166:A:ASP:H | 2 | 0.17 | 0.0 | 0.17 |
| (1,2466) | 1:118:A:ILE:H | 1:140:A:ILE:HA | 2 | 0.17 | 0.04 | 0.17 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD11 | 2 | 0.17 | 0.04 | 0.17 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD12 | 2 | 0.17 | 0.04 | 0.17 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD13 | 2 | 0.17 | 0.04 | 0.17 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD21 | 2 | 0.17 | 0.04 | 0.17 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD22 | 2 | 0.17 | 0.04 | 0.17 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD23 | 2 | 0.17 | 0.04 | 0.17 |
| (1,1582) | 1:201:A:ILE:HG21 | 1:205:A:LYS:HB3 | 2 | 0.16 | 0.04 | 0.16 |
| (1,1582) | 1:201:A:ILE:HG22 | 1:205:A:LYS:HB3 | 2 | 0.16 | 0.04 | 0.16 |
| (1,1582) | 1:201:A:ILE:HG23 | 1:205:A:LYS:HB3 | 2 | 0.16 | 0.04 | 0.16 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD11 | 2 | 0.16 | 0.02 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,815) | 1:117:A:VAL:HG11 | 1:118:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,815) | 1:117:A:VAL:HG12 | 1:118:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,815) | 1:117:A:VAL:HG13 | 1:118:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3155) | 1:56:A:ALA:HB1 | 1:69:A:PHE:HD1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3155) | 1:56:A:ALA:HB1 | 1:69:A:PHE:HD2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3155) | 1:56:A:ALA:HB2 | 1:69:A:PHE:HD1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3155) | 1:56:A:ALA:HB2 | 1:69:A:PHE:HD2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3155) | 1:56:A:ALA:HB3 | 1:69:A:PHE:HD1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3155) | 1:56:A:ALA:HB3 | 1:69:A:PHE:HD2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,2194) | 1:58:A:HIS:H | 1:71:A:GLY:HA2 | 2 | 0.16 | 0.05 | 0.16 |
| (1,2920) | 1:166:A:ASP:HA | 1:195:A:ASN:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,3753) | 1:112:A:TYR:H | 1:120:A:LYS:HD2 | 2 | 0.16 | 0.04 | 0.16 |
| (1,3753) | 1:112:A:TYR:H | 1:120:A:LYS:HD3 | 2 | 0.16 | 0.04 | 0.16 |
| (1,3830) | 1:126:A:ALA:HA | 1:133:A:TRP:HB2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3830) | 1:126:A:ALA:HA | 1:133:A:TRP:HB3 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2611) | 1:116:A:GLN:H | 1:143:A:VAL:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,3289) | 2:4:B:LYS:HB2 | 2:5:B:PRO:HD3 | 2 | 0.15 | 0.03 | 0.15 |
| (1,3289) | 2:4:B:LYS:HB3 | 2:5:B:PRO:HD3 | 2 | 0.15 | 0.03 | 0.15 |
| (1,535) | 1:99:A:GLU:HB3 | 1:100:A:PRO:HD3 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1085) | 1:140:A:ILE:HD11 | 1:149:A:ALA:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,1085) | 1:140:A:ILE:HD12 | 1:149:A:ALA:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,1085) | 1:140:A:ILE:HD13 | 1:149:A:ALA:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,1097) | 1:140:A:ILE:HG21 | 1:151:A:ALA:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,1097) | 1:140:A:ILE:HG22 | 1:151:A:ALA:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,1097) | 1:140:A:ILE:HG23 | 1:151:A:ALA:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD11 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD12 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD13 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD23 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD11 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD12 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD13 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD23 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD11 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD12 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD13 | 2 | 0.15 | 0.0 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD23 | 2 | 0.15 | 0.0 | 0.15 |
| (1,2344) | 1:86:A:GLU:HG2 | 1:87:A:VAL:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,3023) | 1:191:A:THR:H | 1:219:A:THR:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,547) | 1:107:A:LEU:HA | 1:107:A:LEU:HG | 2 | 0.14 | 0.03 | 0.14 |
| (1,630) | 1:98:A:PRO:HA | 1:99:A:GLU:HG2 | 2 | 0.14 | 0.03 | 0.14 |
| (1,630) | 1:98:A:PRO:HA | 1:99:A:GLU:HG3 | 2 | 0.14 | 0.03 | 0.14 |
| (1,2856) | 1:142:A:THR:HG21 | 1:182:A:HIS:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,2856) | 1:142:A:THR:HG22 | 1:182:A:HIS:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,2856) | 1:142:A:THR:HG23 | 1:182:A:HIS:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,3451) | 2:6:B:VAL:HG21 | 2:8:B:ILE:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,3451) | 2:6:B:VAL:HG22 | 2:8:B:ILE:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,3451) | 2:6:B:VAL:HG23 | 2:8:B:ILE:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,245) | 1:63:A:TYR:HA | 1:64:A:PRO:HG2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1656) | 1:192:A:ILE:HD11 | 1:220:A:LEU:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,1656) | 1:192:A:ILE:HD12 | 1:220:A:LEU:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,1656) | 1:192:A:ILE:HD13 | 1:220:A:LEU:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB1 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB1 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB1 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2311) | 1:82:A:LEU:H | 1:112:A:TYR:HD1 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2311) | 1:82:A:LEU:H | 1:112:A:TYR:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2882) | 1:187:A:MET:H | 1:187:A:MET:HG2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1570) | 1:184:A:ILE:HG21 | 1:216:A:LEU:HA | 2 | 0.13 | 0.01 | 0.13 |
| (1,1570) | 1:184:A:ILE:HG22 | 1:216:A:LEU:HA | 2 | 0.13 | 0.01 | 0.13 |
| (1,1570) | 1:184:A:ILE:HG23 | 1:216:A:LEU:HA | 2 | 0.13 | 0.01 | 0.13 |
| (1,2143) | 1:50:A:LEU:H | 1:51:A:PRO:HD2 | 2 | 0.13 | 0.03 | 0.13 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD11 | 2 | 0.13 | 0.01 | 0.13 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD12 | 2 | 0.13 | 0.01 | 0.13 |

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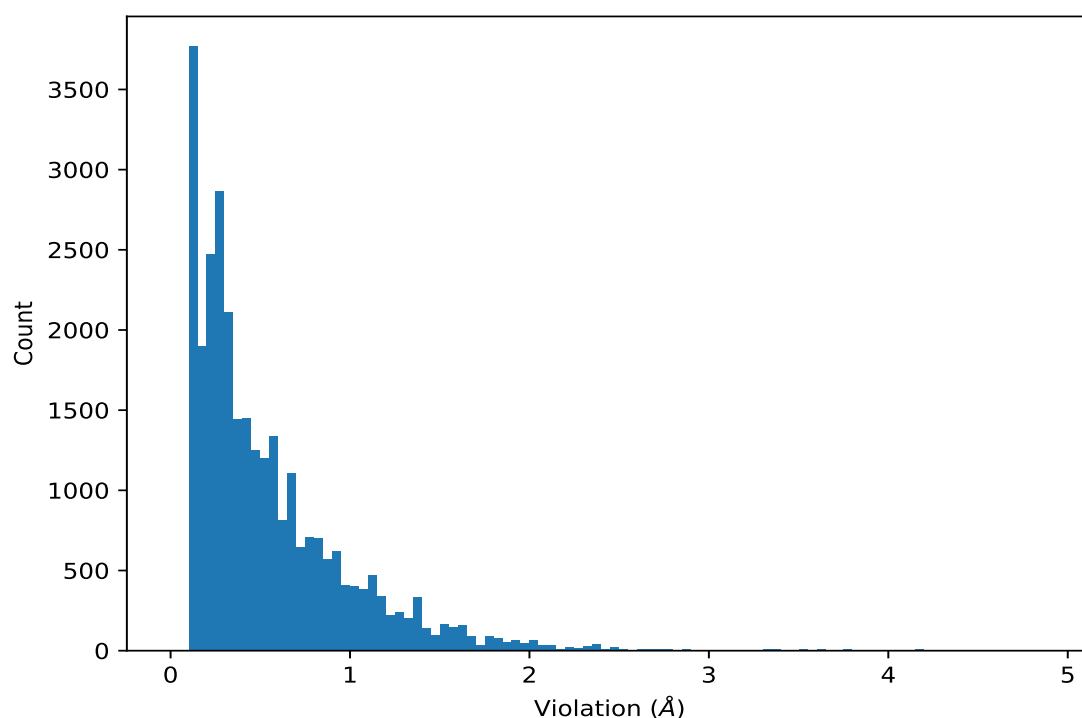
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD13 | 2 | 0.13 | 0.01 | 0.13 |
| (1,3156) | 1:125:A:TRP:H | 1:135:A:PHE:HD1 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3156) | 1:125:A:TRP:H | 1:135:A:PHE:HD2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3707) | 1:102:A:ARG:HG2 | 1:103:A:THR:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3707) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,1201) | 1:209:A:LEU:H | 1:210:A:LYS:HE2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1201) | 1:209:A:LEU:H | 1:210:A:LYS:HE3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,911) | 1:125:A:TRP:HA | 1:134:A:VAL:HB | 2 | 0.11 | 0.01 | 0.11 |
| (1,3178) | 1:170:A:PHE:HA | 1:170:A:PHE:HD1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3178) | 1:170:A:PHE:HA | 1:170:A:PHE:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1724) | 1:167:A:ASP:HA | 1:196:A:ASN:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,2083) | 1:223:A:THR:HB | 1:224:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2083) | 1:223:A:THR:HB | 1:224:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2110) | 1:56:A:ALA:HB1 | 1:73:A:VAL:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,2110) | 1:56:A:ALA:HB2 | 1:73:A:VAL:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,2110) | 1:56:A:ALA:HB3 | 1:73:A:VAL:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,1173) | 1:151:A:ALA:HA | 1:152:A:LYS:HA | 2 | 0.1 | 0.0 | 0.1 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 2 | 4.9 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 2 | 4.9 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 20 | 4.86 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 20 | 4.86 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 14 | 4.63 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 14 | 4.63 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 2 | 4.5 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 2 | 4.5 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 6 | 4.48 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 6 | 4.48 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 17 | 4.38 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 17 | 4.38 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 20 | 4.33 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 20 | 4.33 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 17 | 4.32 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 17 | 4.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 20 | 4.24 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 20 | 4.24 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 14 | 4.22 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 14 | 4.22 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 11 | 4.19 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 11 | 4.19 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 2 | 4.19 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 2 | 4.19 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 16 | 4.18 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 16 | 4.18 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 2 | 4.18 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 2 | 4.18 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 11 | 4.15 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 11 | 4.15 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 20 | 4.09 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 20 | 4.09 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 6 | 4.07 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 6 | 4.07 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 14 | 4.05 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 14 | 4.05 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 2 | 4.02 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 2 | 4.02 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 2 | 4.02 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 2 | 4.02 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 2 | 4.02 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 2 | 4.02 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 6 | 3.95 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 6 | 3.95 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 13 | 3.92 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 13 | 3.92 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 16 | 3.91 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 16 | 3.91 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 6 | 3.9 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 6 | 3.9 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 17 | 3.9 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 14 | 3.89 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 14 | 3.89 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 6 | 3.76 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 6 | 3.75 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 6 | 3.75 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 6 | 3.75 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 6 | 3.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 6 | 3.75 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 6 | 3.75 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 2 | 3.66 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 2 | 3.66 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 17 | 3.65 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 17 | 3.65 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 7 | 3.64 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 6 | 3.62 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 6 | 3.62 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 6 | 3.62 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 6 | 3.62 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 6 | 3.62 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 6 | 3.62 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 16 | 3.57 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 11 | 3.53 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 11 | 3.53 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 6 | 3.52 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 6 | 3.52 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 17 | 3.51 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 17 | 3.51 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 20 | 3.5 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 16 | 3.49 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 16 | 3.49 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 16 | 3.47 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 16 | 3.47 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 8 | 3.45 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 1 | 3.42 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 1 | 3.42 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 18 | 3.42 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 2 | 3.41 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 19 | 3.39 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 19 | 3.39 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 11 | 3.38 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 11 | 3.38 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 13 | 3.38 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 13 | 3.38 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 2 | 3.37 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 2 | 3.37 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 10 | 3.37 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 17 | 3.35 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 9 | 3.33 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 9 | 3.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 6 | 3.33 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 9 | 3.32 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 9 | 3.32 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 9 | 3.32 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 9 | 3.32 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 9 | 3.32 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 9 | 3.32 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 15 | 3.3 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 13 | 3.28 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 7 | 3.27 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 16 | 3.24 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 10 | 3.23 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 10 | 3.23 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 8 | 3.18 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 20 | 3.18 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 2 | 3.15 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 18 | 3.13 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 6 | 3.11 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 6 | 3.11 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 3 | 3.1 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 3 | 3.1 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 15 | 3.06 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 17 | 3.06 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 4 | 3.03 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 4 | 3.03 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 13 | 2.98 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 19 | 2.97 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 19 | 2.97 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 13 | 2.96 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 13 | 2.96 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 2 | 2.92 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 2 | 2.92 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 20 | 2.89 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 20 | 2.89 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 10 | 2.89 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 10 | 2.89 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 7 | 2.88 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 7 | 2.88 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 7 | 2.88 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 10 | 2.85 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 9 | 2.81 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 9 | 2.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 10 | 2.79 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 9 | 2.79 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 9 | 2.79 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 18 | 2.78 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 18 | 2.78 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 6 | 2.77 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 7 | 2.77 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 1 | 2.74 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 1 | 2.74 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 7 | 2.74 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 9 | 2.72 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 9 | 2.72 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 3 | 2.71 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 3 | 2.71 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 9 | 2.71 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 9 | 2.71 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 1 | 2.7 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 1 | 2.7 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 16 | 2.7 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 2 | 2.69 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 2 | 2.69 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 20 | 2.68 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 9 | 2.68 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 9 | 2.68 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 9 | 2.68 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 1 | 2.67 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 1 | 2.67 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 6 | 2.67 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 12 | 2.66 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 12 | 2.66 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 13 | 2.65 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 8 | 2.65 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 20 | 2.63 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 20 | 2.63 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 2 | 2.63 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 6 | 2.61 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 6 | 2.61 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 14 | 2.61 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 14 | 2.61 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 18 | 2.61 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 13 | 2.58 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 13 | 2.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 9 | 2.57 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 6 | 2.56 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 6 | 2.56 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 15 | 2.56 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 19 | 2.54 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 18 | 2.54 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 9 | 2.54 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 9 | 2.54 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 9 | 2.54 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 18 | 2.54 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 14 | 2.52 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 2 | 2.5 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 2 | 2.5 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 6 | 2.49 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 6 | 2.49 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 8 | 2.48 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 8 | 2.48 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 16 | 2.48 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 16 | 2.48 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 16 | 2.48 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 15 | 2.47 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 15 | 2.47 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 9 | 2.46 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 9 | 2.46 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 7 | 2.46 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 7 | 2.46 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 7 | 2.46 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 7 | 2.46 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 10 | 2.45 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 10 | 2.45 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 10 | 2.45 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 10 | 2.45 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 10 | 2.45 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 10 | 2.45 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 9 | 2.45 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 1 | 2.44 |
| (1,20) | 1:47:A:THR:HG21 | 1:50:A:LEU:HA | 9 | 2.44 |
| (1,20) | 1:47:A:THR:HG22 | 1:50:A:LEU:HA | 9 | 2.44 |
| (1,20) | 1:47:A:THR:HG23 | 1:50:A:LEU:HA | 9 | 2.44 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG21 | 6 | 2.41 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG22 | 6 | 2.41 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG23 | 6 | 2.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG21 | 6 | 2.41 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG22 | 6 | 2.41 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG23 | 6 | 2.41 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 9 | 2.4 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 9 | 2.39 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE1 | 2 | 2.38 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE2 | 2 | 2.38 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE3 | 2 | 2.38 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE1 | 2 | 2.38 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE2 | 2 | 2.38 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE3 | 2 | 2.38 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 16 | 2.38 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 9 | 2.38 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 9 | 2.38 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 9 | 2.38 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 7 | 2.38 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 7 | 2.38 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 5 | 2.38 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 5 | 2.38 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 1 | 2.38 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 3 | 2.37 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 3 | 2.37 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 12 | 2.37 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 5 | 2.36 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 5 | 2.36 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 5 | 2.36 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 6 | 2.36 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 17 | 2.36 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 10 | 2.35 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 10 | 2.35 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 10 | 2.35 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 20 | 2.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 20 | 2.35 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE1 | 6 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE2 | 6 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE3 | 6 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE1 | 6 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE2 | 6 | 2.34 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE3 | 6 | 2.34 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 7 | 2.34 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 6 | 2.33 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 11 | 2.32 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 7 | 2.32 |
| (1,897) | 1:123:A:LYS:HE2 | 1:136:A:TYR:HB3 | 4 | 2.32 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 17 | 2.31 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 17 | 2.31 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 19 | 2.31 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 19 | 2.31 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 15 | 2.29 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 15 | 2.29 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 15 | 2.29 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 9 | 2.28 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 9 | 2.28 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 13 | 2.28 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 13 | 2.28 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 2 | 2.28 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 2 | 2.28 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 9 | 2.28 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 9 | 2.28 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 18 | 2.28 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 18 | 2.28 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 18 | 2.28 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 13 | 2.27 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 17 | 2.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 17 | 2.24 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 17 | 2.24 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 18 | 2.24 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 18 | 2.24 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 6 | 2.24 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 6 | 2.24 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 13 | 2.24 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 15 | 2.24 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 15 | 2.24 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 8 | 2.23 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 11 | 2.22 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 11 | 2.22 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 18 | 2.22 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 10 | 2.22 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 10 | 2.21 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 10 | 2.21 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 3 | 2.21 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 1 | 2.21 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 1 | 2.21 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 1 | 2.21 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 18 | 2.2 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 18 | 2.2 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 12 | 2.2 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 6 | 2.19 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG2 | 17 | 2.19 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG3 | 17 | 2.19 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 9 | 2.17 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 12 | 2.17 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 12 | 2.17 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 19 | 2.16 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 19 | 2.16 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 20 | 2.14 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 20 | 2.14 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 20 | 2.14 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 13 | 2.14 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 8 | 2.13 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 8 | 2.13 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 8 | 2.13 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 12 | 2.13 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 10 | 2.13 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 20 | 2.13 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 20 | 2.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 2 | 2.12 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 2 | 2.12 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 10 | 2.12 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 3 | 2.11 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 20 | 2.1 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 20 | 2.1 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 12 | 2.1 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 12 | 2.1 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 15 | 2.1 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 7 | 2.1 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 7 | 2.1 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 10 | 2.1 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 4 | 2.1 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 4 | 2.1 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 4 | 2.1 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 18 | 2.09 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 18 | 2.09 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 4 | 2.09 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 4 | 2.09 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 8 | 2.09 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 8 | 2.09 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 8 | 2.09 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 18 | 2.09 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 18 | 2.09 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 18 | 2.09 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 2 | 2.09 |
| (1,1403) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG3 | 7 | 2.09 |
| (1,1403) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG3 | 7 | 2.09 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 3 | 2.08 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 3 | 2.08 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 9 | 2.08 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 9 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 9 | 2.08 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 12 | 2.07 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 12 | 2.07 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 12 | 2.07 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 12 | 2.07 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 12 | 2.07 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 12 | 2.07 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 14 | 2.07 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 10 | 2.07 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 10 | 2.07 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 14 | 2.07 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 14 | 2.07 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 14 | 2.07 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 4 | 2.06 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 4 | 2.06 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 4 | 2.06 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 7 | 2.05 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 7 | 2.05 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 4 | 2.05 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 4 | 2.05 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 4 | 2.05 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 4 | 2.05 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 19 | 2.05 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 19 | 2.05 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 19 | 2.05 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 19 | 2.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 16 | 2.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 16 | 2.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 16 | 2.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 17 | 2.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 17 | 2.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 17 | 2.05 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 16 | 2.04 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 16 | 2.04 |
| (1,2122) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 5 | 2.04 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 14 | 2.04 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 14 | 2.04 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 11 | 2.04 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 11 | 2.04 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 11 | 2.04 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 1 | 2.03 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 1 | 2.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 20 | 2.02 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 20 | 2.02 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 10 | 2.02 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 10 | 2.02 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 10 | 2.02 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 1 | 2.02 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 1 | 2.02 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 1 | 2.02 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 14 | 2.01 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 8 | 2.0 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 6 | 2.0 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 6 | 2.0 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 6 | 2.0 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 1 | 2.0 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 1 | 2.0 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 17 | 2.0 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 17 | 2.0 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 17 | 2.0 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 2 | 2.0 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 2 | 2.0 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 2 | 2.0 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 2 | 2.0 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 2 | 2.0 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 2 | 2.0 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 18 | 2.0 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 18 | 2.0 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 18 | 2.0 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 4 | 1.99 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 4 | 1.99 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 14 | 1.99 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 14 | 1.99 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 14 | 1.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 17 | 1.99 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 17 | 1.99 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 3 | 1.99 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 18 | 1.99 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 18 | 1.99 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 14 | 1.98 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 14 | 1.98 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 11 | 1.98 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 11 | 1.98 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 11 | 1.98 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 9 | 1.98 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 9 | 1.98 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 4 | 1.98 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 5 | 1.98 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 19 | 1.98 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 7 | 1.98 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 7 | 1.98 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 7 | 1.98 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 2 | 1.98 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 2 | 1.98 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 2 | 1.98 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 3 | 1.97 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 3 | 1.97 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 17 | 1.97 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 17 | 1.97 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 14 | 1.97 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 9 | 1.97 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 15 | 1.97 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 5 | 1.97 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 5 | 1.97 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 5 | 1.97 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 5 | 1.97 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 5 | 1.97 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 20 | 1.97 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 14 | 1.96 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 14 | 1.96 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 14 | 1.96 |
| (1,615) | 1:94:A:ALA:H | 1:97:A:GLN:HG2 | 8 | 1.96 |
| (1,600) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG3 | 6 | 1.96 |
| (1,600) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG3 | 6 | 1.96 |
| (1,600) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG3 | 6 | 1.96 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 3 | 1.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 3 | 1.95 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 7 | 1.95 |
| (1,1403) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG3 | 1 | 1.95 |
| (1,1403) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG3 | 1 | 1.95 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 1 | 1.94 |
| (1,2123) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 5 | 1.94 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 2 | 1.94 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 2 | 1.94 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 11 | 1.94 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 11 | 1.94 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 11 | 1.94 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 7 | 1.94 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 20 | 1.94 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 5 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 5 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 5 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 5 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 5 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 5 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 14 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 14 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 14 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 14 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 14 | 1.93 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 14 | 1.93 |
| (1,2217) | 1:62:A:ASP:H | 1:66:A:ASP:HB2 | 12 | 1.93 |
| (1,876) | 1:122:A:PRO:HG3 | 1:123:A:LYS:HD3 | 4 | 1.93 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 4 | 1.93 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 4 | 1.93 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 4 | 1.93 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 10 | 1.93 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 10 | 1.93 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 10 | 1.93 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 17 | 1.93 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 20 | 1.93 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 20 | 1.93 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 20 | 1.93 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 16 | 1.92 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 16 | 1.92 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 16 | 1.92 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 10 | 1.92 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 10 | 1.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 5 | 1.92 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 7 | 1.92 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 15 | 1.92 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 18 | 1.92 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 16 | 1.91 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 16 | 1.91 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 18 | 1.91 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 15 | 1.91 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 16 | 1.91 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 2 | 1.91 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 2 | 1.91 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 2 | 1.91 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 20 | 1.91 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 20 | 1.91 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 20 | 1.91 |
| (1,1403) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG3 | 12 | 1.91 |
| (1,1403) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG3 | 12 | 1.91 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 7 | 1.91 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 7 | 1.91 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 7 | 1.91 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 11 | 1.9 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 11 | 1.9 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 11 | 1.9 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 15 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 1 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 1 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 1 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 6 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 6 | 1.9 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 6 | 1.9 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 2 | 1.9 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 5 | 1.89 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 5 | 1.89 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 14 | 1.89 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 14 | 1.89 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 20 | 1.89 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 20 | 1.89 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 20 | 1.89 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 16 | 1.89 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 16 | 1.89 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 5 | 1.89 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 5 | 1.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 5 | 1.89 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 13 | 1.88 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 18 | 1.88 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 8 | 1.88 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 8 | 1.88 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 16 | 1.88 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 19 | 1.87 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 19 | 1.87 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 17 | 1.87 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 17 | 1.87 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 18 | 1.87 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 20 | 1.87 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 20 | 1.87 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 20 | 1.87 |
| (1,1002) | 1:123:A:LYS:HD3 | 1:136:A:TYR:HB3 | 4 | 1.87 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 6 | 1.87 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 7 | 1.86 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 7 | 1.86 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 7 | 1.86 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 7 | 1.86 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 7 | 1.86 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 7 | 1.86 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 17 | 1.86 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 11 | 1.86 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 1 | 1.86 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 1 | 1.86 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 1 | 1.86 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 4 | 1.85 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 14 | 1.85 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 16 | 1.85 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 16 | 1.85 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 16 | 1.85 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 14 | 1.84 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 14 | 1.84 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 11 | 1.84 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 11 | 1.84 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 2 | 1.84 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 2 | 1.84 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 7 | 1.84 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 7 | 1.84 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 1 | 1.84 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 1 | 1.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 1 | 1.84 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 1 | 1.84 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 1 | 1.84 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 1 | 1.84 |
| (1,3076) | 1:196:A:ASN:HD22 | 1:225:A:LYS:H | 19 | 1.84 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 13 | 1.84 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 11 | 1.84 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 11 | 1.84 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 6 | 1.84 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 6 | 1.84 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 8 | 1.84 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 14 | 1.83 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 14 | 1.83 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 19 | 1.83 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 17 | 1.83 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 14 | 1.83 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 14 | 1.83 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 14 | 1.83 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 12 | 1.83 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 12 | 1.83 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 5 | 1.83 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 5 | 1.83 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 5 | 1.83 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE1 | 9 | 1.82 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE2 | 9 | 1.82 |
| (1,3351) | 2:10:B:TYR:HD1 | 2:21:B:MET:HE3 | 9 | 1.82 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE1 | 9 | 1.82 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE2 | 9 | 1.82 |
| (1,3351) | 2:10:B:TYR:HD2 | 2:21:B:MET:HE3 | 9 | 1.82 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 8 | 1.82 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 8 | 1.82 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 8 | 1.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 7 | 1.82 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 2 | 1.81 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 20 | 1.81 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 4 | 1.81 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 4 | 1.81 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 4 | 1.81 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 19 | 1.81 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 3 | 1.81 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 12 | 1.81 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 8 | 1.8 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 8 | 1.8 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 8 | 1.8 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 8 | 1.8 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 3 | 1.8 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 11 | 1.8 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 16 | 1.8 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 5 | 1.8 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 5 | 1.8 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 6 | 1.8 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 12 | 1.8 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 11 | 1.8 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 11 | 1.8 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 11 | 1.8 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 9 | 1.79 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 9 | 1.79 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 7 | 1.79 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 7 | 1.79 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 19 | 1.79 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 15 | 1.79 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 15 | 1.79 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 16 | 1.79 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 9 | 1.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 9 | 1.79 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 9 | 1.79 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 12 | 1.78 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 12 | 1.78 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 12 | 1.78 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 12 | 1.78 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 12 | 1.78 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 12 | 1.78 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 4 | 1.78 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 4 | 1.78 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 16 | 1.78 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 20 | 1.78 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 17 | 1.78 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 17 | 1.78 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 17 | 1.78 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 18 | 1.78 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 18 | 1.78 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 18 | 1.78 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 4 | 1.78 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 8 | 1.77 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 8 | 1.77 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 17 | 1.77 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 18 | 1.77 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 2 | 1.77 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 2 | 1.77 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 17 | 1.77 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 17 | 1.77 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 17 | 1.77 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 18 | 1.77 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 18 | 1.77 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 18 | 1.77 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 8 | 1.77 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 8 | 1.77 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 8 | 1.77 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 17 | 1.76 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 17 | 1.76 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 13 | 1.76 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 13 | 1.76 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 13 | 1.76 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 13 | 1.76 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 13 | 1.76 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 13 | 1.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 6 | 1.76 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 6 | 1.76 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 16 | 1.76 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 16 | 1.76 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 10 | 1.76 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 11 | 1.76 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 11 | 1.76 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 11 | 1.76 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 12 | 1.76 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 12 | 1.76 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 12 | 1.76 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 12 | 1.76 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 12 | 1.76 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 12 | 1.76 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 2 | 1.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 2 | 1.75 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 5 | 1.75 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 5 | 1.75 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 10 | 1.75 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 8 | 1.75 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 8 | 1.75 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 8 | 1.75 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 13 | 1.74 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 20 | 1.74 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 20 | 1.74 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 20 | 1.74 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 13 | 1.74 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 10 | 1.73 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 10 | 1.73 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 5 | 1.73 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 5 | 1.73 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 5 | 1.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 5 | 1.73 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 5 | 1.73 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 5 | 1.73 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 20 | 1.73 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 20 | 1.73 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 6 | 1.73 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 13 | 1.73 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 17 | 1.72 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 17 | 1.72 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 9 | 1.72 |
| (1,232) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 7 | 1.72 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 20 | 1.72 |
| (1,20) | 1:47:A:THR:HG21 | 1:50:A:LEU:HA | 18 | 1.72 |
| (1,20) | 1:47:A:THR:HG22 | 1:50:A:LEU:HA | 18 | 1.72 |
| (1,20) | 1:47:A:THR:HG23 | 1:50:A:LEU:HA | 18 | 1.72 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 1 | 1.71 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 17 | 1.71 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 11 | 1.71 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 18 | 1.71 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 18 | 1.71 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 2 | 1.71 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 2 | 1.71 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 2 | 1.71 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 11 | 1.7 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 11 | 1.7 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 11 | 1.7 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 11 | 1.7 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 11 | 1.7 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 11 | 1.7 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 6 | 1.7 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 6 | 1.7 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 6 | 1.7 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 6 | 1.7 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 6 | 1.7 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 6 | 1.7 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 4 | 1.7 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 4 | 1.7 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 12 | 1.7 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 12 | 1.7 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 11 | 1.7 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 11 | 1.7 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 11 | 1.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 17 | 1.7 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 17 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 6 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 6 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 6 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 9 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 9 | 1.7 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 9 | 1.7 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD11 | 18 | 1.7 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD12 | 18 | 1.7 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD13 | 18 | 1.7 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG2 | 6 | 1.69 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG3 | 6 | 1.69 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 5 | 1.69 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 5 | 1.69 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 5 | 1.69 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 5 | 1.69 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 5 | 1.69 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 5 | 1.69 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 12 | 1.69 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 12 | 1.69 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 3 | 1.69 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 9 | 1.69 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 4 | 1.69 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 4 | 1.69 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 4 | 1.69 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 4 | 1.69 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 4 | 1.69 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 2 | 1.69 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 16 | 1.68 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 16 | 1.68 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 16 | 1.68 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 16 | 1.68 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 16 | 1.68 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 16 | 1.68 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 11 | 1.68 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 11 | 1.68 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 16 | 1.68 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 16 | 1.68 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 16 | 1.68 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 10 | 1.68 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 10 | 1.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 10 | 1.68 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 2 | 1.68 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 2 | 1.68 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 16 | 1.67 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 16 | 1.67 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 16 | 1.67 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 16 | 1.67 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 16 | 1.67 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 16 | 1.67 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 6 | 1.67 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 6 | 1.67 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 9 | 1.67 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 16 | 1.67 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 2 | 1.67 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 8 | 1.67 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 4 | 1.67 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 8 | 1.67 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 8 | 1.67 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 8 | 1.67 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 7 | 1.67 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 7 | 1.67 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 7 | 1.66 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 7 | 1.66 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 7 | 1.66 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 7 | 1.66 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 7 | 1.66 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 7 | 1.66 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 5 | 1.66 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 14 | 1.66 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 14 | 1.66 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 14 | 1.66 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 5 | 1.65 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 5 | 1.65 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 5 | 1.65 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 5 | 1.65 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 5 | 1.65 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 5 | 1.65 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 12 | 1.65 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 12 | 1.65 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 12 | 1.65 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 12 | 1.65 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 9 | 1.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 9 | 1.65 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 11 | 1.65 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 11 | 1.65 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 17 | 1.65 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 17 | 1.65 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 15 | 1.64 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 15 | 1.64 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 7 | 1.64 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 7 | 1.64 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 11 | 1.64 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 9 | 1.64 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 16 | 1.64 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 16 | 1.64 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 16 | 1.64 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 4 | 1.64 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 11 | 1.64 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 17 | 1.64 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 10 | 1.63 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 10 | 1.63 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 10 | 1.63 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 10 | 1.63 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 10 | 1.63 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 10 | 1.63 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 18 | 1.63 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 9 | 1.63 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 9 | 1.63 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 19 | 1.63 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 1 | 1.63 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 1 | 1.63 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 1 | 1.63 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 5 | 1.63 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 5 | 1.63 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 5 | 1.63 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 7 | 1.63 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 7 | 1.63 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 7 | 1.63 |
| (1,156) | 1:60:A:LYS:HE2 | 1:70:A:THR:HG21 | 17 | 1.63 |
| (1,156) | 1:60:A:LYS:HE2 | 1:70:A:THR:HG22 | 17 | 1.63 |
| (1,156) | 1:60:A:LYS:HE2 | 1:70:A:THR:HG23 | 17 | 1.63 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG2 | 5 | 1.62 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG3 | 5 | 1.62 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 2 | 1.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 2 | 1.62 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 2 | 1.62 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 2 | 1.62 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 2 | 1.62 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 2 | 1.62 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 17 | 1.62 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 17 | 1.62 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 18 | 1.62 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 18 | 1.62 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 20 | 1.62 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 20 | 1.62 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 3 | 1.62 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 9 | 1.62 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 9 | 1.62 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 9 | 1.62 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 18 | 1.62 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 18 | 1.62 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 18 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 6 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 6 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 6 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 7 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 7 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 7 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 9 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 9 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 9 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 10 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 10 | 1.62 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 10 | 1.62 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 6 | 1.62 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 6 | 1.62 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 6 | 1.62 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 7 | 1.61 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 7 | 1.61 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 7 | 1.61 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 7 | 1.61 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 7 | 1.61 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 7 | 1.61 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 16 | 1.61 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 16 | 1.61 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 13 | 1.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 13 | 1.61 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 20 | 1.61 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 13 | 1.61 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 13 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 8 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 8 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 8 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 10 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 10 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 10 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 16 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 16 | 1.61 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 16 | 1.61 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 2 | 1.61 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 2 | 1.61 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 2 | 1.61 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 20 | 1.61 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 20 | 1.61 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 20 | 1.61 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 1 | 1.61 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 1 | 1.61 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 1 | 1.61 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 8 | 1.61 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 8 | 1.61 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 8 | 1.61 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 7 | 1.61 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 6 | 1.61 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 6 | 1.61 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 6 | 1.61 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 4 | 1.61 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 4 | 1.61 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 4 | 1.61 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 3 | 1.61 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 3 | 1.61 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 3 | 1.61 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 3 | 1.61 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 3 | 1.61 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 3 | 1.61 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 2 | 1.6 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 2 | 1.6 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 6 | 1.6 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 5 | 1.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 5 | 1.6 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 17 | 1.6 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 17 | 1.6 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 17 | 1.6 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 17 | 1.6 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 17 | 1.6 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 17 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 4 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 4 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 4 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 5 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 5 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 5 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 11 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 11 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 11 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 17 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 17 | 1.6 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 17 | 1.6 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 16 | 1.6 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 2 | 1.6 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 14 | 1.59 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 14 | 1.59 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 9 | 1.59 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 9 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 6 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 6 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 6 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 7 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 7 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 7 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 14 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 14 | 1.59 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 14 | 1.59 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 5 | 1.59 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 5 | 1.59 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 5 | 1.59 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 16 | 1.59 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 16 | 1.59 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 18 | 1.59 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 18 | 1.59 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 18 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 19 | 1.59 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 19 | 1.59 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 19 | 1.59 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 7 | 1.58 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 7 | 1.58 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 15 | 1.58 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 15 | 1.58 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 8 | 1.58 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 8 | 1.58 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 8 | 1.58 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 8 | 1.58 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 8 | 1.58 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 8 | 1.58 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 8 | 1.58 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 16 | 1.58 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 5 | 1.58 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 18 | 1.58 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 18 | 1.58 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 18 | 1.58 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 2 | 1.58 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 2 | 1.58 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 2 | 1.58 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 20 | 1.58 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 20 | 1.58 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 20 | 1.58 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 17 | 1.58 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 17 | 1.58 |
| (1,615) | 1:94:A:ALA:H | 1:97:A:GLN:HG2 | 4 | 1.58 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 14 | 1.58 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 14 | 1.58 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 14 | 1.58 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 8 | 1.57 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 8 | 1.57 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 8 | 1.57 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 8 | 1.57 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 8 | 1.57 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 8 | 1.57 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 2 | 1.57 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 2 | 1.57 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 2 | 1.57 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 2 | 1.57 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 5 | 1.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 14 | 1.57 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 14 | 1.57 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 19 | 1.57 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 2 | 1.57 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 18 | 1.57 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 5 | 1.57 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 5 | 1.57 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 5 | 1.57 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 8 | 1.57 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 8 | 1.57 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 8 | 1.57 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 16 | 1.57 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 16 | 1.57 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 16 | 1.57 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 16 | 1.57 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 16 | 1.57 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 16 | 1.57 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 11 | 1.56 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 11 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 6 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 6 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 6 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 6 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 6 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 6 | 1.56 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 19 | 1.56 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 19 | 1.56 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 15 | 1.56 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 9 | 1.56 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 9 | 1.56 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 9 | 1.56 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 13 | 1.56 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 13 | 1.56 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 13 | 1.56 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 9 | 1.56 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 9 | 1.56 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 9 | 1.56 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 9 | 1.56 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 9 | 1.56 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 9 | 1.56 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 16 | 1.56 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 16 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 16 | 1.56 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 16 | 1.56 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 16 | 1.56 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 16 | 1.56 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 7 | 1.56 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 7 | 1.56 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 9 | 1.56 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 20 | 1.56 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 20 | 1.56 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 13 | 1.56 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 13 | 1.56 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 13 | 1.56 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 16 | 1.55 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 16 | 1.55 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 16 | 1.55 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 16 | 1.55 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 16 | 1.55 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 16 | 1.55 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 10 | 1.55 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 10 | 1.55 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 10 | 1.55 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 10 | 1.55 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 10 | 1.55 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 10 | 1.55 |
| (1,3426) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 17 | 1.55 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 17 | 1.55 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 17 | 1.55 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 17 | 1.55 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 17 | 1.55 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 17 | 1.55 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 17 | 1.55 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 2 | 1.55 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 10 | 1.55 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 10 | 1.55 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 11 | 1.55 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 11 | 1.55 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 17 | 1.55 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 4 | 1.55 |
| (1,1411) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB2 | 1 | 1.55 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 2 | 1.55 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 5 | 1.55 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 5 | 1.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 5 | 1.55 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 17 | 1.54 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 11 | 1.54 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 15 | 1.54 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 18 | 1.54 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 18 | 1.54 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 18 | 1.54 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 5 | 1.54 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 6 | 1.54 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 7 | 1.54 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 7 | 1.54 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 7 | 1.54 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 18 | 1.53 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 18 | 1.53 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 18 | 1.53 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 18 | 1.53 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 18 | 1.53 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 18 | 1.53 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 13 | 1.53 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 13 | 1.53 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 5 | 1.53 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 5 | 1.53 |
| (1,2888) | 1:116:A:GLN:HE21 | 1:188:A:GLY:H | 1 | 1.53 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 5 | 1.53 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 5 | 1.53 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 5 | 1.53 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 10 | 1.53 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 10 | 1.53 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 10 | 1.53 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 8 | 1.53 |
| (1,20) | 1:47:A:THR:HG21 | 1:50:A:LEU:HA | 7 | 1.53 |
| (1,20) | 1:47:A:THR:HG22 | 1:50:A:LEU:HA | 7 | 1.53 |
| (1,20) | 1:47:A:THR:HG23 | 1:50:A:LEU:HA | 7 | 1.53 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD21 | 7 | 1.53 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD22 | 7 | 1.53 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD23 | 7 | 1.53 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 1 | 1.52 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 1 | 1.52 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 1 | 1.52 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 1 | 1.52 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 1 | 1.52 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 1 | 1.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 9 | 1.52 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 9 | 1.52 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 11 | 1.52 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 11 | 1.52 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 19 | 1.52 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 19 | 1.52 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 19 | 1.52 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 19 | 1.52 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 16 | 1.52 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 13 | 1.52 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 19 | 1.52 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 15 | 1.52 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 15 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 1 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 1 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 1 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 2 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 2 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 2 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 14 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 14 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 14 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 17 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 17 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 17 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 20 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 20 | 1.52 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 20 | 1.52 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 8 | 1.52 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 8 | 1.52 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 8 | 1.52 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 8 | 1.52 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 8 | 1.52 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 8 | 1.52 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 14 | 1.52 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 14 | 1.52 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 14 | 1.52 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 14 | 1.52 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 14 | 1.52 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 14 | 1.52 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 10 | 1.51 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 10 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 20 | 1.51 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 20 | 1.51 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 1 | 1.51 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 1 | 1.51 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 20 | 1.51 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 20 | 1.51 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 20 | 1.51 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 20 | 1.51 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 20 | 1.51 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 20 | 1.51 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 8 | 1.51 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 8 | 1.51 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 4 | 1.51 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 4 | 1.51 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 4 | 1.51 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 4 | 1.51 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 4 | 1.51 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 4 | 1.51 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 7 | 1.51 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 7 | 1.51 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 1 | 1.51 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 14 | 1.51 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 20 | 1.51 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 1 | 1.51 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 12 | 1.51 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 13 | 1.51 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 17 | 1.51 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 17 | 1.51 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 16 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 16 | 1.51 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 16 | 1.51 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 12 | 1.51 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 12 | 1.51 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 12 | 1.51 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 20 | 1.51 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 20 | 1.51 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 20 | 1.51 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG2 | 2 | 1.5 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG3 | 2 | 1.5 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 1 | 1.5 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 12 | 1.5 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 12 | 1.5 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 12 | 1.5 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 18 | 1.5 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 18 | 1.5 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 18 | 1.5 |
| (1,3079) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 7 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 6 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 6 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 6 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 7 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 7 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 7 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 8 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 8 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 8 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 9 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 9 | 1.5 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 9 | 1.5 |
| (1,1411) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB2 | 7 | 1.5 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 15 | 1.5 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 20 | 1.49 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 20 | 1.49 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 20 | 1.49 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 20 | 1.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 20 | 1.49 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 20 | 1.49 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 13 | 1.49 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 13 | 1.49 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 5 | 1.49 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 2 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 4 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 4 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 4 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 11 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 11 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 11 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 16 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 16 | 1.49 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 16 | 1.49 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 10 | 1.49 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 10 | 1.49 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 10 | 1.49 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 15 | 1.49 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 13 | 1.48 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 4 | 1.48 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 1 | 1.48 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 4 | 1.48 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 18 | 1.48 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 18 | 1.48 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 18 | 1.48 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 17 | 1.48 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 5 | 1.48 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 1 | 1.48 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 1 | 1.48 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 1 | 1.48 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 1 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 1 | 1.48 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 1 | 1.48 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 1 | 1.48 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 1 | 1.48 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 1 | 1.48 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 5 | 1.48 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 5 | 1.48 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 5 | 1.48 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 5 | 1.48 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 5 | 1.48 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 5 | 1.48 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 5 | 1.48 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 3 | 1.48 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 3 | 1.48 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 3 | 1.48 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 3 | 1.47 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 3 | 1.47 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 4 | 1.47 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 12 | 1.47 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 12 | 1.47 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 12 | 1.47 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 16 | 1.47 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 17 | 1.47 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 7 | 1.47 |
| (1,232) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 5 | 1.47 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 16 | 1.47 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE1 | 2 | 1.46 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE2 | 2 | 1.46 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE3 | 2 | 1.46 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE1 | 2 | 1.46 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE2 | 2 | 1.46 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE3 | 2 | 1.46 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 17 | 1.46 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 17 | 1.46 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 19 | 1.46 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 19 | 1.46 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 1 | 1.46 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 1 | 1.46 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 1 | 1.46 |
| (1,613) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG2 | 8 | 1.46 |
| (1,613) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG2 | 8 | 1.46 |
| (1,613) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG2 | 8 | 1.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 13 | 1.46 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 13 | 1.46 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 13 | 1.46 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 2 | 1.46 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 2 | 1.46 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 2 | 1.46 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 3 | 1.45 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 6 | 1.45 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 13 | 1.45 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 13 | 1.45 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 1 | 1.45 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 13 | 1.45 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 13 | 1.45 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 13 | 1.45 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 3 | 1.45 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 3 | 1.45 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 3 | 1.45 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 13 | 1.45 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 13 | 1.45 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 13 | 1.45 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 2 | 1.45 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 2 | 1.45 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 2 | 1.45 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 8 | 1.45 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 8 | 1.45 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 8 | 1.45 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 7 | 1.45 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 4 | 1.45 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 17 | 1.44 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 2 | 1.44 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 2 | 1.44 |
| (1,2122) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 19 | 1.44 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 8 | 1.44 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 6 | 1.44 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 6 | 1.44 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 20 | 1.44 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 20 | 1.44 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 20 | 1.44 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 4 | 1.44 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 4 | 1.44 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 4 | 1.44 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 4 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 4 | 1.44 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 4 | 1.44 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 4 | 1.44 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 4 | 1.44 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 4 | 1.44 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 3 | 1.44 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 3 | 1.44 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 3 | 1.44 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 3 | 1.43 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 3 | 1.43 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 3 | 1.43 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 3 | 1.43 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 3 | 1.43 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 3 | 1.43 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 20 | 1.43 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 20 | 1.43 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 12 | 1.43 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 12 | 1.43 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 12 | 1.43 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 5 | 1.43 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 12 | 1.43 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 12 | 1.43 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 12 | 1.43 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 18 | 1.43 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 5 | 1.43 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 5 | 1.43 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 5 | 1.43 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 17 | 1.43 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 9 | 1.42 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 9 | 1.42 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 9 | 1.42 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 9 | 1.42 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 9 | 1.42 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 9 | 1.42 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 11 | 1.42 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 11 | 1.42 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 3 | 1.42 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 16 | 1.42 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 9 | 1.42 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 16 | 1.42 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 4 | 1.42 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 4 | 1.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 4 | 1.42 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 15 | 1.42 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 15 | 1.42 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 15 | 1.42 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 7 | 1.42 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 7 | 1.42 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 14 | 1.42 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 14 | 1.42 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 14 | 1.42 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 11 | 1.42 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 11 | 1.42 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 11 | 1.42 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 11 | 1.42 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 11 | 1.42 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 11 | 1.42 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 19 | 1.42 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG21 | 2 | 1.42 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG22 | 2 | 1.42 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG23 | 2 | 1.42 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG21 | 2 | 1.42 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG22 | 2 | 1.42 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG23 | 2 | 1.42 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 11 | 1.42 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 11 | 1.42 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 11 | 1.42 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD11 | 9 | 1.42 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD12 | 9 | 1.42 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD13 | 9 | 1.42 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 5 | 1.41 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 5 | 1.41 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 1 | 1.41 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 1 | 1.41 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 5 | 1.41 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 5 | 1.41 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 11 | 1.41 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 11 | 1.41 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 11 | 1.41 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 11 | 1.41 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 11 | 1.41 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 11 | 1.41 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 4 | 1.41 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 4 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 14 | 1.41 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 14 | 1.41 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 13 | 1.41 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 13 | 1.41 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 19 | 1.41 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 2 | 1.41 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 7 | 1.41 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 20 | 1.41 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 6 | 1.41 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 16 | 1.41 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 16 | 1.41 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 11 | 1.41 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 11 | 1.41 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 20 | 1.41 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 20 | 1.41 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 20 | 1.41 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 3 | 1.41 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 16 | 1.41 |
| (1,12) | 1:47:A:THR:HB | 1:50:A:LEU:HG | 18 | 1.41 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 19 | 1.4 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 19 | 1.4 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 19 | 1.4 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 19 | 1.4 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 19 | 1.4 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 19 | 1.4 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 11 | 1.4 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 12 | 1.4 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 2 | 1.4 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 2 | 1.4 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 3 | 1.4 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 3 | 1.4 |
| (1,3046) | 1:196:A:ASN:HD21 | 1:225:A:LYS:H | 4 | 1.4 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 3 | 1.4 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 2 | 1.4 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 2 | 1.4 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 2 | 1.4 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 2 | 1.4 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 2 | 1.4 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 2 | 1.4 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 15 | 1.4 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 5 | 1.4 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 14 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 14 | 1.4 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 14 | 1.4 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 6 | 1.4 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 6 | 1.4 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 6 | 1.4 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 6 | 1.4 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 6 | 1.4 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 6 | 1.4 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 18 | 1.4 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 18 | 1.4 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 18 | 1.4 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 18 | 1.4 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 18 | 1.4 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 18 | 1.4 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 1 | 1.4 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 1 | 1.4 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 1 | 1.4 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 1 | 1.4 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 20 | 1.4 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 20 | 1.4 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 20 | 1.4 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 20 | 1.4 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 9 | 1.4 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 10 | 1.4 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 10 | 1.4 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 10 | 1.4 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 14 | 1.39 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 14 | 1.39 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 14 | 1.39 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 14 | 1.39 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 18 | 1.39 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 8 | 1.39 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 8 | 1.39 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 8 | 1.39 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 8 | 1.39 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 8 | 1.39 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 8 | 1.39 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 4 | 1.39 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 4 | 1.39 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 12 | 1.39 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 12 | 1.39 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 20 | 1.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 20 | 1.39 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 14 | 1.39 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 14 | 1.39 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 7 | 1.39 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 10 | 1.39 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 7 | 1.39 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 7 | 1.39 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 8 | 1.39 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 8 | 1.39 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD11 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD12 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD13 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD11 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD12 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD13 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD11 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD12 | 2 | 1.39 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD13 | 2 | 1.39 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 5 | 1.39 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 7 | 1.39 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 7 | 1.39 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 7 | 1.39 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 7 | 1.39 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 7 | 1.39 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 7 | 1.39 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 14 | 1.39 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 14 | 1.39 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 14 | 1.39 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 14 | 1.39 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 17 | 1.39 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 17 | 1.39 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 17 | 1.39 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 17 | 1.39 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 4 | 1.39 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 4 | 1.39 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 4 | 1.39 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 14 | 1.39 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 14 | 1.39 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 3 | 1.38 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 3 | 1.38 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 3 | 1.38 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 3 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 17 | 1.38 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 4 | 1.38 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 4 | 1.38 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 9 | 1.38 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 9 | 1.38 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 9 | 1.38 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 9 | 1.38 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 9 | 1.38 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 9 | 1.38 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 5 | 1.38 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 8 | 1.38 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 16 | 1.38 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 16 | 1.38 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 16 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 10 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 10 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 10 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 10 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 10 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 10 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 17 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 17 | 1.38 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 17 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 17 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 17 | 1.38 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 17 | 1.38 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 4 | 1.38 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 4 | 1.38 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 4 | 1.38 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 4 | 1.38 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 11 | 1.38 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 11 | 1.38 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 11 | 1.38 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 11 | 1.38 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 14 | 1.38 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 14 | 1.38 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 14 | 1.38 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 18 | 1.38 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD11 | 4 | 1.38 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD12 | 4 | 1.38 |
| (1,30) | 1:49:A:ASP:HA | 1:50:A:LEU:HD13 | 4 | 1.38 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 6 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3598) | 1:77:A:GLN:H | 1:82:A:LEU:HD11 | 10 | 1.37 |
| (1,3598) | 1:77:A:GLN:H | 1:82:A:LEU:HD12 | 10 | 1.37 |
| (1,3598) | 1:77:A:GLN:H | 1:82:A:LEU:HD13 | 10 | 1.37 |
| (1,3598) | 1:77:A:GLN:H | 1:82:A:LEU:HD21 | 10 | 1.37 |
| (1,3598) | 1:77:A:GLN:H | 1:82:A:LEU:HD22 | 10 | 1.37 |
| (1,3598) | 1:77:A:GLN:H | 1:82:A:LEU:HD23 | 10 | 1.37 |
| (1,3459) | 2:10:B:TYR:HE1 | 2:21:B:MET:H | 7 | 1.37 |
| (1,3459) | 2:10:B:TYR:HE2 | 2:21:B:MET:H | 7 | 1.37 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 18 | 1.37 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 18 | 1.37 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 14 | 1.37 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 14 | 1.37 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 15 | 1.37 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 15 | 1.37 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 15 | 1.37 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 15 | 1.37 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 15 | 1.37 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 15 | 1.37 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 1 | 1.37 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 1 | 1.37 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 10 | 1.37 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 19 | 1.37 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 9 | 1.37 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 9 | 1.37 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 9 | 1.37 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 10 | 1.37 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 10 | 1.37 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 10 | 1.37 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 4 | 1.37 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 4 | 1.37 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 1 | 1.37 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 1 | 1.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 2 | 1.37 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 2 | 1.37 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 2 | 1.37 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 2 | 1.37 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 10 | 1.37 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 10 | 1.37 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 10 | 1.37 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 10 | 1.37 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 7 | 1.37 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 7 | 1.37 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 7 | 1.37 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 7 | 1.37 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 7 | 1.37 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 7 | 1.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 19 | 1.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 19 | 1.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 19 | 1.37 |
| (1,3603) | 1:77:A:GLN:HB3 | 1:82:A:LEU:HD11 | 10 | 1.36 |
| (1,3603) | 1:77:A:GLN:HB3 | 1:82:A:LEU:HD12 | 10 | 1.36 |
| (1,3603) | 1:77:A:GLN:HB3 | 1:82:A:LEU:HD13 | 10 | 1.36 |
| (1,3603) | 1:77:A:GLN:HB3 | 1:82:A:LEU:HD21 | 10 | 1.36 |
| (1,3603) | 1:77:A:GLN:HB3 | 1:82:A:LEU:HD22 | 10 | 1.36 |
| (1,3603) | 1:77:A:GLN:HB3 | 1:82:A:LEU:HD23 | 10 | 1.36 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 16 | 1.36 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 16 | 1.36 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 16 | 1.36 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 16 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 18 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 18 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 18 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 18 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 18 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 18 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 19 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 19 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 19 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 19 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 19 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 19 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 20 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 20 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 20 | 1.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 20 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 20 | 1.36 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 20 | 1.36 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 13 | 1.36 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 1 | 1.36 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 1 | 1.36 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 20 | 1.36 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 11 | 1.36 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 17 | 1.36 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 17 | 1.36 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 19 | 1.36 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 19 | 1.36 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 19 | 1.36 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 2 | 1.36 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 2 | 1.36 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 2 | 1.36 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 19 | 1.36 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 5 | 1.36 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 5 | 1.36 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 5 | 1.36 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 5 | 1.36 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 5 | 1.36 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 5 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 5 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 5 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 5 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 5 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 6 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 6 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 6 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 6 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 8 | 1.36 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 8 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 8 | 1.36 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 8 | 1.36 |
| (1,541) | 1:94:A:ALA:H | 1:97:A:GLN:HG3 | 11 | 1.36 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 19 | 1.36 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 18 | 1.36 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 18 | 1.36 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 4 | 1.36 |
| (1,242) | 1:142:A:THR:HG21 | 1:146:A:PRO:HD2 | 12 | 1.36 |
| (1,242) | 1:142:A:THR:HG22 | 1:146:A:PRO:HD2 | 12 | 1.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,242) | 1:142:A:THR:HG23 | 1:146:A:PRO:HD2 | 12 | 1.36 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 12 | 1.36 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 12 | 1.36 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 12 | 1.36 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 12 | 1.36 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 12 | 1.36 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 12 | 1.36 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 6 | 1.36 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 6 | 1.36 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 5 | 1.35 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 5 | 1.35 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 9 | 1.35 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 9 | 1.35 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 3 | 1.35 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 3 | 1.35 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 1 | 1.35 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 1 | 1.35 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 11 | 1.35 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 11 | 1.35 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 14 | 1.35 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 14 | 1.35 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 9 | 1.35 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 9 | 1.35 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 4 | 1.35 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 2 | 1.35 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 5 | 1.35 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 14 | 1.35 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 14 | 1.35 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 14 | 1.35 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 14 | 1.35 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 14 | 1.35 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 14 | 1.35 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 7 | 1.35 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 7 | 1.35 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 7 | 1.35 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 7 | 1.35 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 16 | 1.35 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 16 | 1.35 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 16 | 1.35 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 16 | 1.35 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 1 | 1.35 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 1 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 1 | 1.35 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 1 | 1.35 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 1 | 1.35 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 1 | 1.35 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 18 | 1.35 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 18 | 1.35 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 1 | 1.35 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG21 | 6 | 1.35 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG22 | 6 | 1.35 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG23 | 6 | 1.35 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG21 | 6 | 1.35 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG22 | 6 | 1.35 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG23 | 6 | 1.35 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 5 | 1.35 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 20 | 1.34 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 20 | 1.34 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 8 | 1.34 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 8 | 1.34 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 17 | 1.34 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 18 | 1.34 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 18 | 1.34 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 11 | 1.34 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 6 | 1.34 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 6 | 1.34 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 5 | 1.34 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 15 | 1.34 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 15 | 1.34 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 15 | 1.34 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 18 | 1.34 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 18 | 1.34 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 16 | 1.34 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 1 | 1.34 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 1 | 1.34 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 1 | 1.34 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 13 | 1.34 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 13 | 1.34 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 2 | 1.34 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 2 | 1.34 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 2 | 1.34 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 2 | 1.34 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 2 | 1.34 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 2 | 1.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 9 | 1.34 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 9 | 1.34 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 9 | 1.34 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 9 | 1.34 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 17 | 1.34 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 17 | 1.34 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 17 | 1.34 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 20 | 1.34 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 2 | 1.34 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 2 | 1.34 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 2 | 1.34 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 11 | 1.33 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 11 | 1.33 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 11 | 1.33 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 11 | 1.33 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 18 | 1.33 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 18 | 1.33 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 18 | 1.33 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 18 | 1.33 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 18 | 1.33 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 18 | 1.33 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 10 | 1.33 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 10 | 1.33 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 10 | 1.33 |
| (1,3496) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HA | 16 | 1.33 |
| (1,3496) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HA | 16 | 1.33 |
| (1,3496) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HA | 16 | 1.33 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 18 | 1.33 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 18 | 1.33 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 7 | 1.33 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 3 | 1.33 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 6 | 1.33 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 20 | 1.33 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 20 | 1.33 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 9 | 1.33 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 9 | 1.33 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 18 | 1.33 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 18 | 1.33 |
| (1,1411) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB2 | 12 | 1.33 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 17 | 1.33 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 14 | 1.33 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 18 | 1.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 1 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 1 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 1 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 15 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 15 | 1.32 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 15 | 1.32 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 3 | 1.32 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 3 | 1.32 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 5 | 1.32 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 5 | 1.32 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 16 | 1.32 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 16 | 1.32 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 2 | 1.32 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 2 | 1.32 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 6 | 1.32 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 7 | 1.32 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 7 | 1.32 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 7 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 11 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 11 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 11 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 12 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 12 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 12 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 15 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 15 | 1.32 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 15 | 1.32 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 6 | 1.32 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 9 | 1.32 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 10 | 1.32 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 15 | 1.32 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 14 | 1.32 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 14 | 1.32 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 18 | 1.32 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 18 | 1.32 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 18 | 1.32 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 18 | 1.32 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 5 | 1.32 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 10 | 1.32 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 7 | 1.32 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 7 | 1.32 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 7 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 3 | 1.32 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 10 | 1.31 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 10 | 1.31 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 7 | 1.31 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 7 | 1.31 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 7 | 1.31 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 7 | 1.31 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 7 | 1.31 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 7 | 1.31 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 10 | 1.31 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 3 | 1.31 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 20 | 1.31 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 20 | 1.31 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 4 | 1.31 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 4 | 1.31 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 10 | 1.31 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 10 | 1.31 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 10 | 1.31 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 10 | 1.31 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 10 | 1.31 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 10 | 1.31 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 8 | 1.31 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 10 | 1.31 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 5 | 1.31 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 5 | 1.31 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 1 | 1.31 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 1 | 1.31 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 1 | 1.31 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 9 | 1.31 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 2 | 1.31 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 14 | 1.31 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 20 | 1.31 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 19 | 1.31 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 19 | 1.31 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 19 | 1.31 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 19 | 1.31 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 2 | 1.31 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 2 | 1.31 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 2 | 1.31 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 19 | 1.31 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 19 | 1.31 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 19 | 1.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 6 | 1.31 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 6 | 1.31 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 6 | 1.31 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 6 | 1.31 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 6 | 1.31 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 6 | 1.31 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 7 | 1.31 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 3 | 1.31 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 5 | 1.31 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 19 | 1.31 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 19 | 1.31 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 13 | 1.3 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 13 | 1.3 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 5 | 1.3 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 5 | 1.3 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 5 | 1.3 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 5 | 1.3 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 18 | 1.3 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 18 | 1.3 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 18 | 1.3 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 3 | 1.3 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 3 | 1.3 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 12 | 1.3 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 12 | 1.3 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 10 | 1.3 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 10 | 1.3 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 18 | 1.3 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 6 | 1.3 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 6 | 1.3 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 16 | 1.3 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 10 | 1.3 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 10 | 1.3 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 10 | 1.3 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 3 | 1.3 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 20 | 1.3 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 20 | 1.3 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 20 | 1.3 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 20 | 1.3 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 20 | 1.3 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 20 | 1.3 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 12 | 1.3 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 12 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 8 | 1.3 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 5 | 1.3 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 5 | 1.3 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 5 | 1.3 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 5 | 1.3 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 5 | 1.3 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 5 | 1.3 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 2 | 1.29 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 2 | 1.29 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 15 | 1.29 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 15 | 1.29 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 15 | 1.29 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 15 | 1.29 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 15 | 1.29 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 15 | 1.29 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 5 | 1.29 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 5 | 1.29 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 10 | 1.29 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 10 | 1.29 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 12 | 1.29 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 12 | 1.29 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 20 | 1.29 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 7 | 1.29 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 7 | 1.29 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 20 | 1.29 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 11 | 1.29 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 11 | 1.29 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 13 | 1.29 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 13 | 1.29 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 17 | 1.29 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 17 | 1.29 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 14 | 1.29 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 14 | 1.29 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 14 | 1.29 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 13 | 1.29 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 13 | 1.29 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 13 | 1.29 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 19 | 1.29 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 19 | 1.29 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 19 | 1.29 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 18 | 1.29 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 18 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 18 | 1.29 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 5 | 1.29 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 5 | 1.29 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 5 | 1.29 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 8 | 1.29 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 3 | 1.29 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 3 | 1.29 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 3 | 1.29 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 3 | 1.29 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 11 | 1.29 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 11 | 1.29 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 11 | 1.29 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 13 | 1.29 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 13 | 1.29 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 13 | 1.29 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 13 | 1.29 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 13 | 1.29 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 13 | 1.29 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 10 | 1.28 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 10 | 1.28 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 5 | 1.28 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 5 | 1.28 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 5 | 1.28 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 5 | 1.28 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 5 | 1.28 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 5 | 1.28 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 10 | 1.28 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 15 | 1.28 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 15 | 1.28 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 9 | 1.28 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 9 | 1.28 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 6 | 1.28 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 14 | 1.28 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 1 | 1.28 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 3 | 1.28 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 3 | 1.28 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 3 | 1.28 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 18 | 1.28 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 18 | 1.28 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 4 | 1.28 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 4 | 1.28 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 3 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 3 | 1.28 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 3 | 1.28 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 1 | 1.28 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 1 | 1.28 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 1 | 1.28 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 8 | 1.28 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 8 | 1.28 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 8 | 1.28 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 16 | 1.28 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 16 | 1.28 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 16 | 1.28 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 4 | 1.28 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 13 | 1.28 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 20 | 1.28 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 20 | 1.28 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 20 | 1.28 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 20 | 1.28 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 12 | 1.28 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 12 | 1.28 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 13 | 1.28 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 14 | 1.28 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 4 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 13 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 13 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 13 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 13 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 13 | 1.27 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 13 | 1.27 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 14 | 1.27 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 14 | 1.27 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 12 | 1.27 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 12 | 1.27 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 16 | 1.27 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 16 | 1.27 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 3 | 1.27 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 3 | 1.27 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 11 | 1.27 |
| (1,2122) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 3 | 1.27 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 12 | 1.27 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 12 | 1.27 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 6 | 1.27 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 6 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 6 | 1.27 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 9 | 1.27 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 9 | 1.27 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 9 | 1.27 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 11 | 1.27 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 16 | 1.27 |
| (1,1406) | 1:174:A:GLU:HG2 | 1:175:A:ASN:HA | 17 | 1.27 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 9 | 1.27 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 10 | 1.27 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 10 | 1.27 |
| (1,955) | 1:131:A:LYS:HE2 | 1:160:A:GLY:HA2 | 20 | 1.27 |
| (1,955) | 1:131:A:LYS:HE3 | 1:160:A:GLY:HA2 | 20 | 1.27 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD11 | 20 | 1.27 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD12 | 20 | 1.27 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD13 | 20 | 1.27 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD21 | 20 | 1.27 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD22 | 20 | 1.27 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD23 | 20 | 1.27 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 20 | 1.27 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 20 | 1.27 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 2 | 1.27 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 2 | 1.27 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 2 | 1.27 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 2 | 1.27 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 14 | 1.27 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 14 | 1.27 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 14 | 1.27 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 14 | 1.27 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 16 | 1.27 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 16 | 1.27 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 16 | 1.27 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 16 | 1.27 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 13 | 1.27 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 13 | 1.27 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 13 | 1.27 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 13 | 1.27 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 16 | 1.27 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 13 | 1.27 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 5 | 1.27 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 5 | 1.27 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 11 | 1.26 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 11 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 11 | 1.26 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 11 | 1.26 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 11 | 1.26 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 11 | 1.26 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 10 | 1.26 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 10 | 1.26 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 10 | 1.26 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 10 | 1.26 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 10 | 1.26 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 10 | 1.26 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 13 | 1.26 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 13 | 1.26 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 13 | 1.26 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 13 | 1.26 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 12 | 1.26 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 12 | 1.26 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 9 | 1.26 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 9 | 1.26 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 4 | 1.26 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 4 | 1.26 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 4 | 1.26 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 4 | 1.26 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 4 | 1.26 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 4 | 1.26 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 13 | 1.26 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 13 | 1.26 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 3 | 1.26 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 3 | 1.26 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 8 | 1.26 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 8 | 1.26 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 7 | 1.26 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 18 | 1.26 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 8 | 1.26 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 8 | 1.26 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 8 | 1.26 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 8 | 1.26 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 8 | 1.26 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 17 | 1.26 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 17 | 1.26 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 17 | 1.26 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 17 | 1.26 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 11 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 11 | 1.26 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 11 | 1.26 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 17 | 1.26 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 17 | 1.26 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 17 | 1.26 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 7 | 1.26 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 10 | 1.26 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 10 | 1.26 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 13 | 1.25 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 13 | 1.25 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 13 | 1.25 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 13 | 1.25 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 13 | 1.25 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 13 | 1.25 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 13 | 1.25 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 13 | 1.25 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 13 | 1.25 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 1 | 1.25 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 17 | 1.25 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 17 | 1.25 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 6 | 1.25 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 1 | 1.25 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 1 | 1.25 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 16 | 1.25 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 16 | 1.25 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 16 | 1.25 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 11 | 1.25 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 11 | 1.25 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 11 | 1.25 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 11 | 1.25 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 13 | 1.25 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 13 | 1.25 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 13 | 1.25 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 17 | 1.25 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 17 | 1.25 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 18 | 1.25 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 18 | 1.25 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 18 | 1.25 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 18 | 1.25 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 12 | 1.24 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 12 | 1.24 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 12 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 12 | 1.24 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 12 | 1.24 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 12 | 1.24 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 2 | 1.24 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 2 | 1.24 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 2 | 1.24 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 10 | 1.24 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 2 | 1.24 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 2 | 1.24 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 7 | 1.24 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 5 | 1.24 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 5 | 1.24 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 4 | 1.24 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 18 | 1.24 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 19 | 1.24 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 19 | 1.24 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 19 | 1.24 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 10 | 1.24 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 11 | 1.24 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 19 | 1.24 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 19 | 1.24 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 19 | 1.24 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 3 | 1.24 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 3 | 1.24 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 3 | 1.24 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 9 | 1.24 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 9 | 1.24 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 9 | 1.24 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 9 | 1.24 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 4 | 1.24 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 4 | 1.24 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 4 | 1.24 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 1 | 1.24 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 1 | 1.24 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 1 | 1.24 |
| (1,242) | 1:142:A:THR:HG21 | 1:146:A:PRO:HD2 | 19 | 1.24 |
| (1,242) | 1:142:A:THR:HG22 | 1:146:A:PRO:HD2 | 19 | 1.24 |
| (1,242) | 1:142:A:THR:HG23 | 1:146:A:PRO:HD2 | 19 | 1.24 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 8 | 1.24 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 8 | 1.24 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 8 | 1.24 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 7 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 7 | 1.24 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 7 | 1.24 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 6 | 1.23 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 6 | 1.23 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 6 | 1.23 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 6 | 1.23 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 6 | 1.23 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 6 | 1.23 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 8 | 1.23 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 8 | 1.23 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 8 | 1.23 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 8 | 1.23 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 8 | 1.23 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 8 | 1.23 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 3 | 1.23 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 3 | 1.23 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 3 | 1.23 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 3 | 1.23 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 3 | 1.23 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 3 | 1.23 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 15 | 1.23 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 15 | 1.23 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 14 | 1.23 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 14 | 1.23 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 6 | 1.23 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 6 | 1.23 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 15 | 1.23 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 15 | 1.23 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG21 | 5 | 1.23 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG22 | 5 | 1.23 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG23 | 5 | 1.23 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 1 | 1.23 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 3 | 1.23 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 14 | 1.23 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 2 | 1.23 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 17 | 1.23 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 17 | 1.23 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 17 | 1.23 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 18 | 1.23 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 4 | 1.23 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 4 | 1.23 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 4 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 4 | 1.23 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 6 | 1.23 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 6 | 1.23 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 6 | 1.23 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 6 | 1.23 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 12 | 1.23 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 7 | 1.23 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 3 | 1.23 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 3 | 1.23 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 3 | 1.23 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 4 | 1.22 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 4 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 13 | 1.22 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 13 | 1.22 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 12 | 1.22 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 12 | 1.22 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 12 | 1.22 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 12 | 1.22 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 4 | 1.22 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 4 | 1.22 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 8 | 1.22 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 8 | 1.22 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 8 | 1.22 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 8 | 1.22 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 4 | 1.22 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 3 | 1.22 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 2 | 1.22 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 8 | 1.22 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 8 | 1.22 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 8 | 1.22 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 8 | 1.22 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 8 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 8 | 1.22 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 4 | 1.22 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 12 | 1.22 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 13 | 1.22 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 13 | 1.22 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 13 | 1.22 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 5 | 1.22 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 13 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 1 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 1 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 1 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 1 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 5 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 5 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 5 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 5 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 7 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 7 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 7 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 7 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 10 | 1.22 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 10 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 10 | 1.22 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 10 | 1.22 |
| (1,600) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG3 | 15 | 1.22 |
| (1,600) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG3 | 15 | 1.22 |
| (1,600) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG3 | 15 | 1.22 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 11 | 1.22 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 15 | 1.22 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 2 | 1.22 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 2 | 1.22 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 2 | 1.22 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 2 | 1.22 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 2 | 1.22 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 2 | 1.22 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 5 | 1.22 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 5 | 1.22 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 5 | 1.22 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 5 | 1.22 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 5 | 1.22 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 5 | 1.22 |
| (1,4019) | 2:12:B:ASN:HD22 | 2:13:B:ARG:HB2 | 5 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4019) | 2:12:B:ASN:HD22 | 2:13:B:ARG:HB3 | 5 | 1.21 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 13 | 1.21 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 13 | 1.21 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 13 | 1.21 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 13 | 1.21 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 13 | 1.21 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 13 | 1.21 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 17 | 1.21 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 17 | 1.21 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 6 | 1.21 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 6 | 1.21 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 6 | 1.21 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 6 | 1.21 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 12 | 1.21 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 3 | 1.21 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 3 | 1.21 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 3 | 1.21 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 13 | 1.21 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 20 | 1.21 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 20 | 1.21 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 1 | 1.21 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 20 | 1.21 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 4 | 1.21 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 15 | 1.21 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 15 | 1.21 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 15 | 1.21 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 19 | 1.21 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 19 | 1.21 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 19 | 1.21 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 15 | 1.21 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 15 | 1.21 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 18 | 1.21 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 20 | 1.21 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 20 | 1.21 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 20 | 1.21 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 5 | 1.21 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 5 | 1.21 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 5 | 1.21 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 17 | 1.21 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 18 | 1.21 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 12 | 1.21 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 10 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 13 | 1.21 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 13 | 1.21 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 13 | 1.21 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 13 | 1.21 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 13 | 1.21 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 13 | 1.21 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 16 | 1.21 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 16 | 1.21 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 16 | 1.21 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE21 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE22 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE21 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE22 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE21 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE22 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE21 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE22 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE21 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE22 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE21 | 7 | 1.2 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE22 | 7 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 13 | 1.2 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 13 | 1.2 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 6 | 1.2 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 6 | 1.2 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 8 | 1.2 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 6 | 1.2 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 18 | 1.2 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 18 | 1.2 |
| (1,3123) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HE1 | 10 | 1.2 |
| (1,3123) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HE2 | 10 | 1.2 |
| (1,3123) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HE1 | 10 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3123) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HE2 | 10 | 1.2 |
| (1,3123) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HE1 | 10 | 1.2 |
| (1,3123) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HE2 | 10 | 1.2 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 2 | 1.2 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 6 | 1.2 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 6 | 1.2 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 6 | 1.2 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 6 | 1.2 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 6 | 1.2 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 6 | 1.2 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 16 | 1.2 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 16 | 1.2 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 16 | 1.2 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 16 | 1.2 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 16 | 1.2 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 16 | 1.2 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 13 | 1.2 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 17 | 1.2 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD21 | 12 | 1.2 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD22 | 12 | 1.2 |
| (1,1972) | 1:214:A:ALA:HA | 1:216:A:LEU:HD23 | 12 | 1.2 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 10 | 1.2 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 10 | 1.2 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 10 | 1.2 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 19 | 1.2 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 11 | 1.2 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 11 | 1.2 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 11 | 1.2 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 19 | 1.2 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 7 | 1.2 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 6 | 1.2 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 3 | 1.2 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 4 | 1.2 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 6 | 1.2 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 3 | 1.2 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 3 | 1.2 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 3 | 1.2 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 3 | 1.2 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 19 | 1.2 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 19 | 1.2 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 19 | 1.2 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 19 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 16 | 1.2 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 16 | 1.2 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 16 | 1.2 |
| (1,468) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 5 | 1.2 |
| (1,14) | 1:47:A:THR:HB | 1:49:A:ASP:H | 6 | 1.2 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 7 | 1.2 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 7 | 1.2 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 12 | 1.19 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 12 | 1.19 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 13 | 1.19 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 13 | 1.19 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 1 | 1.19 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 1 | 1.19 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 1 | 1.19 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 1 | 1.19 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 1 | 1.19 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 1 | 1.19 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 15 | 1.19 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 8 | 1.19 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 8 | 1.19 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 8 | 1.19 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 8 | 1.19 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 8 | 1.19 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 8 | 1.19 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 11 | 1.19 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 20 | 1.19 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 8 | 1.19 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 8 | 1.19 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 11 | 1.19 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 4 | 1.19 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 8 | 1.19 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 12 | 1.19 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 16 | 1.19 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 8 | 1.19 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 10 | 1.19 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 10 | 1.19 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 4 | 1.19 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 4 | 1.19 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 4 | 1.19 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 15 | 1.19 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 18 | 1.19 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 18 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 18 | 1.19 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 13 | 1.19 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 17 | 1.19 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 17 | 1.19 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 17 | 1.19 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 4 | 1.19 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 4 | 1.19 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 2 | 1.19 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 10 | 1.19 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 8 | 1.19 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 8 | 1.19 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 8 | 1.19 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 5 | 1.19 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 5 | 1.19 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 5 | 1.19 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 9 | 1.19 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 9 | 1.19 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 9 | 1.19 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 9 | 1.19 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 9 | 1.19 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 9 | 1.19 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 9 | 1.19 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 9 | 1.19 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 9 | 1.19 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 4 | 1.18 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 4 | 1.18 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 15 | 1.18 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 15 | 1.18 |
| (1,3406) | 2:8:B:ILE:HD11 | 2:21:B:MET:HG3 | 2 | 1.18 |
| (1,3406) | 2:8:B:ILE:HD12 | 2:21:B:MET:HG3 | 2 | 1.18 |
| (1,3406) | 2:8:B:ILE:HD13 | 2:21:B:MET:HG3 | 2 | 1.18 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 4 | 1.18 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 10 | 1.18 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 10 | 1.18 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 17 | 1.18 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 17 | 1.18 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 4 | 1.18 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 9 | 1.18 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 12 | 1.18 |
| (1,2122) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 13 | 1.18 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 20 | 1.18 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 20 | 1.18 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 20 | 1.18 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 20 | 1.18 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 8 | 1.18 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 11 | 1.18 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 19 | 1.18 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 19 | 1.18 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 17 | 1.18 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 17 | 1.18 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 17 | 1.18 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 4 | 1.18 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 4 | 1.18 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 4 | 1.18 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 5 | 1.18 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 2 | 1.18 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 3 | 1.18 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 6 | 1.18 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 9 | 1.18 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 14 | 1.18 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 20 | 1.18 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 7 | 1.18 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 4 | 1.18 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 13 | 1.18 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 13 | 1.18 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 13 | 1.18 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 13 | 1.18 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 13 | 1.18 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 8 | 1.18 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 8 | 1.18 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 8 | 1.18 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 8 | 1.18 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 8 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 8 | 1.18 |
| (1,482) | 1:82:A:LEU:HG | 1:112:A:TYR:HE1 | 10 | 1.18 |
| (1,482) | 1:82:A:LEU:HG | 1:112:A:TYR:HE2 | 10 | 1.18 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 5 | 1.18 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 5 | 1.18 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 5 | 1.18 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 9 | 1.18 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 9 | 1.18 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 9 | 1.18 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 9 | 1.18 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 9 | 1.18 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 9 | 1.18 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 13 | 1.18 |
| (1,3833) | 1:127:A:ASN:HB2 | 1:130:A:THR:HB | 20 | 1.17 |
| (1,3833) | 1:127:A:ASN:HB3 | 1:130:A:THR:HB | 20 | 1.17 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 12 | 1.17 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 12 | 1.17 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 12 | 1.17 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 12 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 9 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 9 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 9 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 9 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 9 | 1.17 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 9 | 1.17 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 15 | 1.17 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 15 | 1.17 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 7 | 1.17 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD11 | 3 | 1.17 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD12 | 3 | 1.17 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD13 | 3 | 1.17 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD21 | 3 | 1.17 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD22 | 3 | 1.17 |
| (1,3209) | 1:133:A:TRP:HD1 | 1:163:A:LEU:HD23 | 3 | 1.17 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 6 | 1.17 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 6 | 1.17 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 10 | 1.17 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 10 | 1.17 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 17 | 1.17 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 20 | 1.17 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 19 | 1.17 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 9 | 1.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 18 | 1.17 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 20 | 1.17 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 20 | 1.17 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 20 | 1.17 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 17 | 1.17 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 17 | 1.17 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 17 | 1.17 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 10 | 1.17 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 18 | 1.17 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 18 | 1.17 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 18 | 1.17 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD11 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD12 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD13 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD11 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD12 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD13 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD11 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD12 | 3 | 1.17 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD13 | 3 | 1.17 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 7 | 1.17 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 3 | 1.17 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 8 | 1.17 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 8 | 1.17 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 8 | 1.17 |
| (1,896) | 1:123:A:LYS:HE3 | 1:136:A:TYR:HB3 | 7 | 1.17 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 16 | 1.17 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 1 | 1.17 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 1 | 1.17 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 1 | 1.17 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 17 | 1.17 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 17 | 1.17 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 17 | 1.17 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 17 | 1.17 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 17 | 1.17 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 17 | 1.17 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 16 | 1.17 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 16 | 1.17 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 16 | 1.17 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 15 | 1.17 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 15 | 1.17 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 7 | 1.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 7 | 1.17 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 7 | 1.17 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 20 | 1.16 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 20 | 1.16 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 20 | 1.16 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 20 | 1.16 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 20 | 1.16 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 20 | 1.16 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 11 | 1.16 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 11 | 1.16 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 7 | 1.16 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 19 | 1.16 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 19 | 1.16 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 10 | 1.16 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 6 | 1.16 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 6 | 1.16 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 11 | 1.16 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 11 | 1.16 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 2 | 1.16 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 4 | 1.16 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 5 | 1.16 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 6 | 1.16 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 16 | 1.16 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 13 | 1.16 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 13 | 1.16 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 13 | 1.16 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 13 | 1.16 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 13 | 1.16 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 13 | 1.16 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 6 | 1.16 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 9 | 1.16 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 15 | 1.16 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 14 | 1.16 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 14 | 1.16 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 14 | 1.16 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 14 | 1.16 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 14 | 1.16 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 14 | 1.16 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 20 | 1.16 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 20 | 1.16 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 14 | 1.16 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 3 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 3 | 1.16 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 3 | 1.16 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 14 | 1.16 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 3 | 1.16 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 8 | 1.16 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 8 | 1.16 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 8 | 1.16 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 10 | 1.16 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 10 | 1.16 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 10 | 1.16 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 9 | 1.16 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 9 | 1.16 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 9 | 1.16 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 5 | 1.16 |
| (1,12) | 1:47:A:THR:HB | 1:50:A:LEU:HG | 7 | 1.16 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 13 | 1.15 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 13 | 1.15 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 3 | 1.15 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 3 | 1.15 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 1 | 1.15 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 1 | 1.15 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 1 | 1.15 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 1 | 1.15 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 10 | 1.15 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 10 | 1.15 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 10 | 1.15 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 10 | 1.15 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 12 | 1.15 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 12 | 1.15 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 12 | 1.15 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 12 | 1.15 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 12 | 1.15 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 12 | 1.15 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 4 | 1.15 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 10 | 1.15 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 10 | 1.15 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 19 | 1.15 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 19 | 1.15 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 19 | 1.15 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 20 | 1.15 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 8 | 1.15 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 8 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 20 | 1.15 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 20 | 1.15 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 3 | 1.15 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 3 | 1.15 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 7 | 1.15 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 7 | 1.15 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 7 | 1.15 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 2 | 1.15 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 7 | 1.15 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 10 | 1.15 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 5 | 1.15 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 5 | 1.15 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 11 | 1.15 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 11 | 1.15 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 11 | 1.15 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 13 | 1.15 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 13 | 1.15 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 13 | 1.15 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 8 | 1.15 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 2 | 1.15 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 8 | 1.15 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 19 | 1.15 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 1 | 1.15 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 12 | 1.15 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 1 | 1.15 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 1 | 1.15 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 2 | 1.15 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 19 | 1.15 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 19 | 1.15 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 19 | 1.15 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 6 | 1.15 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 6 | 1.15 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 17 | 1.15 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 17 | 1.15 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 17 | 1.15 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 17 | 1.15 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 17 | 1.15 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 17 | 1.15 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 17 | 1.14 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 14 | 1.14 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 3 | 1.14 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 3 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 10 | 1.14 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 10 | 1.14 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 8 | 1.14 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 9 | 1.14 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 9 | 1.14 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 15 | 1.14 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 15 | 1.14 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 20 | 1.14 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 20 | 1.14 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 5 | 1.14 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 7 | 1.14 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 2 | 1.14 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 14 | 1.14 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 17 | 1.14 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 16 | 1.14 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 14 | 1.14 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 14 | 1.14 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 14 | 1.14 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 6 | 1.14 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 18 | 1.14 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 4 | 1.14 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 13 | 1.14 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 16 | 1.14 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 17 | 1.14 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD11 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD12 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD13 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD11 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD12 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD13 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD11 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD12 | 13 | 1.14 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD13 | 13 | 1.14 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 11 | 1.14 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 11 | 1.14 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 11 | 1.14 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 15 | 1.14 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 14 | 1.14 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 2 | 1.14 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 18 | 1.14 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 12 | 1.14 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 12 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 12 | 1.14 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 12 | 1.14 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG2 | 3 | 1.14 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG3 | 3 | 1.14 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 7 | 1.14 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 7 | 1.14 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 7 | 1.14 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 16 | 1.14 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 16 | 1.14 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 16 | 1.14 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 11 | 1.13 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 11 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 20 | 1.13 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 20 | 1.13 |
| (1,3572) | 1:64:A:PRO:HB3 | 1:91:A:GLN:HE21 | 7 | 1.13 |
| (1,3572) | 1:64:A:PRO:HB3 | 1:91:A:GLN:HE22 | 7 | 1.13 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 10 | 1.13 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 10 | 1.13 |
| (1,3437) | 2:12:B:ASN:HB2 | 2:16:B:GLY:H | 13 | 1.13 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 10 | 1.13 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 10 | 1.13 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 19 | 1.13 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 5 | 1.13 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 14 | 1.13 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 20 | 1.13 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 20 | 1.13 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 18 | 1.13 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 18 | 1.13 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 18 | 1.13 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 18 | 1.13 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 18 | 1.13 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 18 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 15 | 1.13 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 13 | 1.13 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 13 | 1.13 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 12 | 1.13 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 12 | 1.13 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 12 | 1.13 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 1 | 1.13 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 16 | 1.13 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 16 | 1.13 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 16 | 1.13 |
| (1,1405) | 1:174:A:GLU:HG3 | 1:175:A:ASN:HA | 11 | 1.13 |
| (1,1404) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG2 | 1 | 1.13 |
| (1,1404) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG2 | 1 | 1.13 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 4 | 1.13 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 16 | 1.13 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 16 | 1.13 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 10 | 1.13 |
| (1,613) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG2 | 6 | 1.13 |
| (1,613) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG2 | 6 | 1.13 |
| (1,613) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG2 | 6 | 1.13 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 6 | 1.13 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 6 | 1.13 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 6 | 1.13 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 16 | 1.13 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 16 | 1.13 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 16 | 1.13 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 16 | 1.13 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 16 | 1.13 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 16 | 1.13 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 14 | 1.13 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 2 | 1.13 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 2 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 19 | 1.13 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 2 | 1.13 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 6 | 1.13 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 10 | 1.13 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 10 | 1.13 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 10 | 1.13 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 10 | 1.13 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 10 | 1.13 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 10 | 1.13 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 9 | 1.12 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 9 | 1.12 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 12 | 1.12 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 12 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 2 | 1.12 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 2 | 1.12 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 5 | 1.12 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 5 | 1.12 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 7 | 1.12 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 7 | 1.12 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 4 | 1.12 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 9 | 1.12 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 9 | 1.12 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 14 | 1.12 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 18 | 1.12 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 18 | 1.12 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 2 | 1.12 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 2 | 1.12 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 2 | 1.12 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 14 | 1.12 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 14 | 1.12 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 14 | 1.12 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 1 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 2 | 1.12 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 9 | 1.12 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 9 | 1.12 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 16 | 1.12 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 16 | 1.12 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 20 | 1.12 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 20 | 1.12 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 20 | 1.12 |
| (1,1574) | 1:184:A:ILE:HG21 | 1:215:A:GLU:HG2 | 15 | 1.12 |
| (1,1574) | 1:184:A:ILE:HG22 | 1:215:A:GLU:HG2 | 15 | 1.12 |
| (1,1574) | 1:184:A:ILE:HG23 | 1:215:A:GLU:HG2 | 15 | 1.12 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 14 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 12 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 12 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 12 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 14 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 14 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 14 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 15 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 15 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 15 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 20 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 20 | 1.12 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 20 | 1.12 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 16 | 1.12 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 16 | 1.12 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 16 | 1.12 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 11 | 1.12 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 20 | 1.12 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 14 | 1.12 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 14 | 1.12 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 14 | 1.12 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 1 | 1.12 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 7 | 1.12 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 7 | 1.12 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 7 | 1.12 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG21 | 5 | 1.12 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG22 | 5 | 1.12 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG23 | 5 | 1.12 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG21 | 5 | 1.12 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG22 | 5 | 1.12 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG23 | 5 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 5 | 1.12 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 5 | 1.12 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 5 | 1.12 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 2 | 1.11 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 2 | 1.11 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 16 | 1.11 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 16 | 1.11 |
| (1,3623) | 1:81:A:ARG:HD2 | 1:83:A:GLN:HG2 | 16 | 1.11 |
| (1,3623) | 1:81:A:ARG:HD3 | 1:83:A:GLN:HG2 | 16 | 1.11 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 4 | 1.11 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 1 | 1.11 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 12 | 1.11 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 12 | 1.11 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 12 | 1.11 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 16 | 1.11 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 16 | 1.11 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 16 | 1.11 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 10 | 1.11 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 10 | 1.11 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 6 | 1.11 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 6 | 1.11 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 15 | 1.11 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 13 | 1.11 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 16 | 1.11 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 19 | 1.11 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 8 | 1.11 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 8 | 1.11 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 8 | 1.11 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 11 | 1.11 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 20 | 1.11 |
| (1,2129) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB3 | 5 | 1.11 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 5 | 1.11 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 20 | 1.11 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 7 | 1.11 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 7 | 1.11 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 10 | 1.11 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 10 | 1.11 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 11 | 1.11 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 11 | 1.11 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 3 | 1.11 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 3 | 1.11 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 3 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 17 | 1.11 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 17 | 1.11 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 1 | 1.11 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 13 | 1.11 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 4 | 1.11 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 8 | 1.11 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 8 | 1.11 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 8 | 1.11 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 18 | 1.11 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 10 | 1.11 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 10 | 1.11 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 10 | 1.11 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 19 | 1.11 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 19 | 1.11 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 19 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 6 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 6 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 6 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 19 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 19 | 1.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 19 | 1.11 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 17 | 1.11 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 19 | 1.11 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 19 | 1.11 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 19 | 1.11 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 19 | 1.11 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB2 | 15 | 1.11 |
| (1,584) | 1:212:A:LYS:HG2 | 1:215:A:GLU:HB3 | 15 | 1.11 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB2 | 15 | 1.11 |
| (1,584) | 1:212:A:LYS:HG3 | 1:215:A:GLU:HB3 | 15 | 1.11 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 2 | 1.11 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 2 | 1.11 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 2 | 1.11 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 2 | 1.11 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 2 | 1.11 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 2 | 1.11 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 10 | 1.11 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 10 | 1.11 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 3 | 1.11 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 3 | 1.11 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 16 | 1.11 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 16 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 16 | 1.11 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 8 | 1.11 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 10 | 1.1 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 10 | 1.1 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 19 | 1.1 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 19 | 1.1 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 19 | 1.1 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 19 | 1.1 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 19 | 1.1 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 19 | 1.1 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 6 | 1.1 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 6 | 1.1 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 20 | 1.1 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 4 | 1.1 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 7 | 1.1 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 7 | 1.1 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 13 | 1.1 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 18 | 1.1 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 18 | 1.1 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 18 | 1.1 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 18 | 1.1 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 18 | 1.1 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 18 | 1.1 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 7 | 1.1 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 7 | 1.1 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 7 | 1.1 |
| (1,1993) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HA | 2 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 2 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 2 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 6 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 6 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 8 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 8 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 14 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 14 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 17 | 1.1 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 17 | 1.1 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 2 | 1.1 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 2 | 1.1 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 3 | 1.1 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 3 | 1.1 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 3 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 7 | 1.1 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 7 | 1.1 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 7 | 1.1 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 7 | 1.1 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 5 | 1.1 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 5 | 1.1 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 5 | 1.1 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 5 | 1.1 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 5 | 1.1 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 5 | 1.1 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 12 | 1.1 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 19 | 1.1 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 19 | 1.1 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 8 | 1.1 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 2 | 1.1 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 2 | 1.1 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 2 | 1.1 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 5 | 1.1 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 5 | 1.1 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 5 | 1.1 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 12 | 1.1 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 1 | 1.1 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 8 | 1.1 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 18 | 1.1 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 18 | 1.1 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 18 | 1.1 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 18 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 8 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 8 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 8 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 8 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 8 | 1.1 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 8 | 1.1 |
| (1,446) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA3 | 15 | 1.1 |
| (1,446) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA3 | 15 | 1.1 |
| (1,446) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA3 | 15 | 1.1 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 17 | 1.1 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 17 | 1.1 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 17 | 1.1 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 6 | 1.1 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 6 | 1.1 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 6 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 5 | 1.1 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG21 | 20 | 1.1 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG22 | 20 | 1.1 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG23 | 20 | 1.1 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG21 | 20 | 1.1 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG22 | 20 | 1.1 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG23 | 20 | 1.1 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 20 | 1.1 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 20 | 1.1 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 20 | 1.1 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 20 | 1.1 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 20 | 1.1 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 20 | 1.1 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 2 | 1.1 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 2 | 1.1 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 2 | 1.1 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 12 | 1.1 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 12 | 1.1 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 12 | 1.1 |
| (1,12) | 1:47:A:THR:HB | 1:50:A:LEU:HG | 9 | 1.1 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD11 | 20 | 1.1 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD12 | 20 | 1.1 |
| (1,11) | 1:47:A:THR:HB | 1:50:A:LEU:HD13 | 20 | 1.1 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 2 | 1.1 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 2 | 1.1 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 1 | 1.09 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 1 | 1.09 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG21 | 8 | 1.09 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG22 | 8 | 1.09 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG23 | 8 | 1.09 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG21 | 8 | 1.09 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG22 | 8 | 1.09 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG23 | 8 | 1.09 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 12 | 1.09 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 12 | 1.09 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 12 | 1.09 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 12 | 1.09 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 12 | 1.09 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 12 | 1.09 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 20 | 1.09 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 20 | 1.09 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 20 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 20 | 1.09 |
| (1,3342) | 2:12:B:ASN:H | 2:18:B:CYS:HA | 13 | 1.09 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 5 | 1.09 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 13 | 1.09 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 7 | 1.09 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 10 | 1.09 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 10 | 1.09 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 17 | 1.09 |
| (1,1404) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG2 | 7 | 1.09 |
| (1,1404) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG2 | 7 | 1.09 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 7 | 1.09 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 7 | 1.09 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 7 | 1.09 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 16 | 1.09 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 6 | 1.09 |
| (1,1212) | 1:153:A:VAL:HB | 1:166:A:ASP:HB3 | 16 | 1.09 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 8 | 1.09 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 8 | 1.09 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 8 | 1.09 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 15 | 1.09 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 15 | 1.09 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 15 | 1.09 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 1 | 1.09 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 1 | 1.09 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 20 | 1.09 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 20 | 1.09 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 20 | 1.09 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 20 | 1.09 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 20 | 1.09 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 20 | 1.09 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 8 | 1.09 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 17 | 1.08 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 17 | 1.08 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 12 | 1.08 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 12 | 1.08 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 12 | 1.08 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 12 | 1.08 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 12 | 1.08 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 12 | 1.08 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 17 | 1.08 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 17 | 1.08 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 17 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 17 | 1.08 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 1 | 1.08 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 1 | 1.08 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 14 | 1.08 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 14 | 1.08 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 14 | 1.08 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 14 | 1.08 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 14 | 1.08 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 19 | 1.08 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 2 | 1.08 |
| (1,2647) | 1:148:A:SER:H | 1:179:A:LEU:HD11 | 19 | 1.08 |
| (1,2647) | 1:148:A:SER:H | 1:179:A:LEU:HD12 | 19 | 1.08 |
| (1,2647) | 1:148:A:SER:H | 1:179:A:LEU:HD13 | 19 | 1.08 |
| (1,2647) | 1:148:A:SER:H | 1:179:A:LEU:HD21 | 19 | 1.08 |
| (1,2647) | 1:148:A:SER:H | 1:179:A:LEU:HD22 | 19 | 1.08 |
| (1,2647) | 1:148:A:SER:H | 1:179:A:LEU:HD23 | 19 | 1.08 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 1 | 1.08 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 5 | 1.08 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 10 | 1.08 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 11 | 1.08 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 11 | 1.08 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 12 | 1.08 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 12 | 1.08 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 12 | 1.08 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 12 | 1.08 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 12 | 1.08 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 5 | 1.08 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 5 | 1.08 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 5 | 1.08 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 18 | 1.08 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 18 | 1.08 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 18 | 1.08 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 9 | 1.08 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 19 | 1.08 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 19 | 1.08 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 19 | 1.08 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 12 | 1.08 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 12 | 1.08 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 12 | 1.08 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 12 | 1.08 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 12 | 1.08 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 12 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 4 | 1.08 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 4 | 1.08 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 4 | 1.08 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 7 | 1.08 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 7 | 1.08 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 15 | 1.08 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 6 | 1.08 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 17 | 1.08 |
| (1,345) | 1:73:A:VAL:HA | 1:87:A:VAL:H | 4 | 1.08 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 5 | 1.08 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 20 | 1.08 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 20 | 1.08 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 20 | 1.08 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 8 | 1.07 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 8 | 1.07 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 19 | 1.07 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 19 | 1.07 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 15 | 1.07 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 15 | 1.07 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE1 | 9 | 1.07 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE2 | 9 | 1.07 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE3 | 9 | 1.07 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE1 | 9 | 1.07 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE2 | 9 | 1.07 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE3 | 9 | 1.07 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 20 | 1.07 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 2 | 1.07 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 13 | 1.07 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 13 | 1.07 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 16 | 1.07 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 16 | 1.07 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 3 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 3 | 1.07 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 3 | 1.07 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 19 | 1.07 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 19 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 1 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 1 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 1 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 1 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 1 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 1 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 20 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 20 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 20 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 20 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 20 | 1.07 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 20 | 1.07 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 8 | 1.07 |
| (1,2229) | 1:66:A:ASP:H | 1:67:A:ALA:H | 6 | 1.07 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 20 | 1.07 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 20 | 1.07 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 3 | 1.07 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 3 | 1.07 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 3 | 1.07 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 1 | 1.07 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 1 | 1.07 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 3 | 1.07 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 3 | 1.07 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 4 | 1.07 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 4 | 1.07 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 2 | 1.07 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 2 | 1.07 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 2 | 1.07 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 6 | 1.07 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 6 | 1.07 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 6 | 1.07 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 8 | 1.07 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 8 | 1.07 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 8 | 1.07 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD11 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD12 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG21 | 1:54:A:ILE:HD13 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD11 | 16 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD12 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG22 | 1:54:A:ILE:HD13 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD11 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD12 | 16 | 1.07 |
| (1,1374) | 1:53:A:THR:HG23 | 1:54:A:ILE:HD13 | 16 | 1.07 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 6 | 1.07 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 10 | 1.07 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 12 | 1.07 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 12 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 7 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 7 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 7 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 16 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 16 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 16 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 18 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 18 | 1.07 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 18 | 1.07 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 14 | 1.07 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 14 | 1.07 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 14 | 1.07 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 7 | 1.07 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 4 | 1.07 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 14 | 1.07 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 19 | 1.07 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 9 | 1.07 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 3 | 1.07 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 3 | 1.07 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 3 | 1.07 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 14 | 1.06 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 14 | 1.06 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 19 | 1.06 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 19 | 1.06 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 1 | 1.06 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 1 | 1.06 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 7 | 1.06 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 7 | 1.06 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 14 | 1.06 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 14 | 1.06 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 1 | 1.06 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 1 | 1.06 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 14 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 6 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 6 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 6 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 6 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 6 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 6 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 7 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 7 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 7 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 7 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 7 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 7 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 11 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 11 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 11 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 11 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 11 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 11 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 12 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 12 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 12 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 12 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 12 | 1.06 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 12 | 1.06 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 13 | 1.06 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 6 | 1.06 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 6 | 1.06 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 6 | 1.06 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG2 | 13 | 1.06 |
| (1,2090) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HG3 | 13 | 1.06 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 18 | 1.06 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 18 | 1.06 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 14 | 1.06 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 11 | 1.06 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 11 | 1.06 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 11 | 1.06 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 14 | 1.06 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 14 | 1.06 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 16 | 1.06 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 16 | 1.06 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 16 | 1.06 |
| (1,1404) | 1:173:A:TYR:HD1 | 1:174:A:GLU:HG2 | 12 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1404) | 1:173:A:TYR:HD2 | 1:174:A:GLU:HG2 | 12 | 1.06 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 11 | 1.06 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 15 | 1.06 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 6 | 1.06 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 5 | 1.06 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 5 | 1.06 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 1 | 1.06 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 13 | 1.06 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 18 | 1.06 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 18 | 1.06 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 18 | 1.06 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 9 | 1.06 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 9 | 1.06 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 9 | 1.06 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 1 | 1.06 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 10 | 1.06 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 6 | 1.06 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 6 | 1.06 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 6 | 1.06 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 18 | 1.06 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 18 | 1.06 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 7 | 1.05 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 7 | 1.05 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 15 | 1.05 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 15 | 1.05 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 15 | 1.05 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 15 | 1.05 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 18 | 1.05 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 18 | 1.05 |
| (1,3834) | 1:127:A:ASN:HB2 | 1:131:A:LYS:H | 20 | 1.05 |
| (1,3834) | 1:127:A:ASN:HB3 | 1:131:A:LYS:H | 20 | 1.05 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG2 | 8 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG3 | 8 | 1.05 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 11 | 1.05 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 11 | 1.05 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 11 | 1.05 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 11 | 1.05 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 11 | 1.05 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 11 | 1.05 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 16 | 1.05 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 20 | 1.05 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 3 | 1.05 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 3 | 1.05 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 19 | 1.05 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 19 | 1.05 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 11 | 1.05 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 14 | 1.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 19 | 1.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 19 | 1.05 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 19 | 1.05 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 18 | 1.05 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 9 | 1.05 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 9 | 1.05 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 9 | 1.05 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 16 | 1.05 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 14 | 1.05 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 14 | 1.05 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 14 | 1.05 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 8 | 1.05 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 8 | 1.05 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 8 | 1.05 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 18 | 1.05 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 20 | 1.05 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 3 | 1.05 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 4 | 1.05 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 13 | 1.05 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 16 | 1.05 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 2 | 1.05 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 2 | 1.05 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 2 | 1.05 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 11 | 1.05 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 11 | 1.05 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 11 | 1.05 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 9 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 9 | 1.05 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 9 | 1.05 |
| (1,897) | 1:123:A:LYS:HE2 | 1:136:A:TYR:HB3 | 7 | 1.05 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 2 | 1.05 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 2 | 1.05 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 2 | 1.05 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 17 | 1.05 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 17 | 1.05 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 17 | 1.05 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 17 | 1.05 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 17 | 1.05 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 17 | 1.05 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 5 | 1.05 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 9 | 1.05 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 19 | 1.05 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 5 | 1.05 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 7 | 1.05 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 7 | 1.05 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 7 | 1.05 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 7 | 1.05 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 7 | 1.05 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 7 | 1.05 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 14 | 1.04 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 5 | 1.04 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 5 | 1.04 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 10 | 1.04 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 19 | 1.04 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 17 | 1.04 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 17 | 1.04 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 4 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 4 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 4 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 4 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 4 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 4 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 8 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 8 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 8 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 8 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 8 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 8 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 13 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 14 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 14 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 14 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 14 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 14 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 14 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 16 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 16 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 16 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 16 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 16 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 16 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 17 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 17 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 17 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 17 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 17 | 1.04 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 17 | 1.04 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 19 | 1.04 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 19 | 1.04 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 19 | 1.04 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 5 | 1.04 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 5 | 1.04 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 5 | 1.04 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 10 | 1.04 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 10 | 1.04 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 6 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 2 | 1.04 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 2 | 1.04 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 2 | 1.04 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 18 | 1.04 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 18 | 1.04 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 18 | 1.04 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 15 | 1.04 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 15 | 1.04 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 15 | 1.04 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 1 | 1.04 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 19 | 1.04 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 5 | 1.04 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 5 | 1.04 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 5 | 1.04 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 11 | 1.04 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 14 | 1.04 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 14 | 1.04 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 14 | 1.04 |
| (1,615) | 1:94:A:ALA:H | 1:97:A:GLN:HG2 | 11 | 1.04 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 1 | 1.04 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 5 | 1.04 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 5 | 1.04 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 5 | 1.04 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 5 | 1.04 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 11 | 1.04 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 11 | 1.04 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 11 | 1.04 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 11 | 1.04 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 11 | 1.04 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 11 | 1.04 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 16 | 1.04 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 8 | 1.03 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 8 | 1.03 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 4 | 1.03 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 4 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 20 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 20 | 1.03 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 20 | 1.03 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 9 | 1.03 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 9 | 1.03 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 17 | 1.03 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 17 | 1.03 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 1 | 1.03 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 10 | 1.03 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 10 | 1.03 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 17 | 1.03 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 14 | 1.03 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 10 | 1.03 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 10 | 1.03 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 10 | 1.03 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 10 | 1.03 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 10 | 1.03 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 10 | 1.03 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 5 | 1.03 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 16 | 1.03 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 8 | 1.03 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 8 | 1.03 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 5 | 1.03 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 1 | 1.03 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 1 | 1.03 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 1 | 1.03 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 6 | 1.03 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 6 | 1.03 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 16 | 1.03 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 2 | 1.03 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 2 | 1.03 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 2 | 1.03 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 13 | 1.03 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 13 | 1.03 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 13 | 1.03 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 2 | 1.03 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 6 | 1.03 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 9 | 1.03 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 6 | 1.03 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 6 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 6 | 1.03 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 14 | 1.03 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 14 | 1.03 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 14 | 1.03 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 8 | 1.03 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 13 | 1.03 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 13 | 1.03 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 13 | 1.03 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 3 | 1.03 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 3 | 1.03 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 3 | 1.03 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 2 | 1.03 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 2 | 1.03 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 9 | 1.03 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 9 | 1.03 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 5 | 1.03 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 5 | 1.03 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 12 | 1.03 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 2 | 1.03 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 2 | 1.02 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 2 | 1.02 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 2 | 1.02 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 2 | 1.02 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 11 | 1.02 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 13 | 1.02 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 15 | 1.02 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 15 | 1.02 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG21 | 13 | 1.02 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG22 | 13 | 1.02 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG23 | 13 | 1.02 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 2 | 1.02 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 18 | 1.02 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 4 | 1.02 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 15 | 1.02 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 15 | 1.02 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 10 | 1.02 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 10 | 1.02 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 10 | 1.02 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 13 | 1.02 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 13 | 1.02 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 20 | 1.02 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 2 | 1.02 |

Continued on next page...

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 2 | 1.02 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 2 | 1.02 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 8 | 1.02 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 12 | 1.02 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 20 | 1.02 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 18 | 1.02 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 18 | 1.02 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 18 | 1.02 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 17 | 1.02 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 11 | 1.02 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 15 | 1.02 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 5 | 1.02 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 5 | 1.02 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 5 | 1.02 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 14 | 1.02 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 2 | 1.02 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 6 | 1.02 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 7 | 1.02 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 7 | 1.02 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 7 | 1.02 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 7 | 1.02 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 7 | 1.02 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 7 | 1.02 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 5 | 1.02 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 5 | 1.02 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 5 | 1.02 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 5 | 1.02 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 15 | 1.02 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 15 | 1.02 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG21 | 3 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG22 | 3 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG23 | 3 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG21 | 3 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG22 | 3 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG23 | 3 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG21 | 14 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG22 | 14 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG23 | 14 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG21 | 14 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG22 | 14 | 1.01 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG23 | 14 | 1.01 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 15 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 15 | 1.01 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 15 | 1.01 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 15 | 1.01 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 13 | 1.01 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 13 | 1.01 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 13 | 1.01 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 8 | 1.01 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 8 | 1.01 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 5 | 1.01 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 5 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 2 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 2 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 2 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 2 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 2 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 2 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 19 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 19 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 19 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 19 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 19 | 1.01 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 19 | 1.01 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 4 | 1.01 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 10 | 1.01 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 20 | 1.01 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 20 | 1.01 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 20 | 1.01 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 6 | 1.01 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 6 | 1.01 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 6 | 1.01 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 12 | 1.01 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 12 | 1.01 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 12 | 1.01 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 5 | 1.01 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 5 | 1.01 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 20 | 1.01 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 5 | 1.01 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 10 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 12 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 12 | 1.01 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 12 | 1.01 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 19 | 1.01 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 19 | 1.01 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 19 | 1.01 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 2 | 1.01 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 2 | 1.01 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 14 | 1.01 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 14 | 1.01 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 14 | 1.01 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 4 | 1.01 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 3 | 1.01 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 3 | 1.01 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 3 | 1.01 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 19 | 1.01 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 19 | 1.01 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 19 | 1.01 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 8 | 1.01 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 8 | 1.01 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 8 | 1.01 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 7 | 1.01 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 8 | 1.01 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 11 | 1.01 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 20 | 1.01 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 20 | 1.01 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 15 | 1.01 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 15 | 1.01 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 15 | 1.01 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 18 | 1.01 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 5 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 5 | 1.0 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 5 | 1.0 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 5 | 1.0 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 5 | 1.0 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 5 | 1.0 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 16 | 1.0 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 16 | 1.0 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 5 | 1.0 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 4 | 1.0 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 4 | 1.0 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 7 | 1.0 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 9 | 1.0 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 9 | 1.0 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 19 | 1.0 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 16 | 1.0 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 16 | 1.0 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 1 | 1.0 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 1 | 1.0 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 8 | 1.0 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 12 | 1.0 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 19 | 1.0 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 13 | 1.0 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 13 | 1.0 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 13 | 1.0 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 6 | 1.0 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 6 | 1.0 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 6 | 1.0 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 19 | 1.0 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 19 | 1.0 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 19 | 1.0 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 4 | 1.0 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 4 | 1.0 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 2 | 1.0 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 2 | 1.0 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 2 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 6 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 6 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 6 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 6 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 6 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 6 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 20 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 20 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 20 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 20 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 20 | 1.0 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 20 | 1.0 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 11 | 1.0 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 10 | 1.0 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 10 | 1.0 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 10 | 1.0 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 10 | 1.0 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 10 | 1.0 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 10 | 1.0 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 10 | 1.0 |
| (1,1140) | 1:94:A:ALA:HB1 | 1:101:A:VAL:H | 1 | 1.0 |
| (1,1140) | 1:94:A:ALA:HB2 | 1:101:A:VAL:H | 1 | 1.0 |
| (1,1140) | 1:94:A:ALA:HB3 | 1:101:A:VAL:H | 1 | 1.0 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 14 | 1.0 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 14 | 1.0 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 14 | 1.0 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 14 | 1.0 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 14 | 1.0 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 2 | 1.0 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 2 | 1.0 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 2 | 1.0 |
| (1,592) | 1:141:A:GLU:HG2 | 1:148:A:SER:HB2 | 7 | 1.0 |
| (1,592) | 1:141:A:GLU:HG2 | 1:148:A:SER:HB3 | 7 | 1.0 |
| (1,592) | 1:141:A:GLU:HG3 | 1:148:A:SER:HB2 | 7 | 1.0 |
| (1,592) | 1:141:A:GLU:HG3 | 1:148:A:SER:HB3 | 7 | 1.0 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD21 | 12 | 1.0 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD22 | 12 | 1.0 |
| (1,558) | 1:184:A:ILE:H | 1:216:A:LEU:HD23 | 12 | 1.0 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,468) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 14 | 1.0 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 4 | 1.0 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 18 | 1.0 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 18 | 1.0 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 18 | 1.0 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 18 | 1.0 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 18 | 1.0 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 18 | 1.0 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 19 | 1.0 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 19 | 1.0 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 19 | 1.0 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 19 | 1.0 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 19 | 1.0 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 19 | 1.0 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 13 | 0.99 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 13 | 0.99 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 13 | 0.99 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 13 | 0.99 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 13 | 0.99 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 13 | 0.99 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 16 | 0.99 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 16 | 0.99 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE1 | 12 | 0.99 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE2 | 12 | 0.99 |
| (1,3349) | 2:10:B:TYR:HE1 | 2:21:B:MET:HE3 | 12 | 0.99 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE1 | 12 | 0.99 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE2 | 12 | 0.99 |
| (1,3349) | 2:10:B:TYR:HE2 | 2:21:B:MET:HE3 | 12 | 0.99 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 17 | 0.99 |
| (1,3097) | 1:58:A:HIS:HE1 | 1:61:A:GLY:H | 9 | 0.99 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 4 | 0.99 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 10 | 0.99 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 18 | 0.99 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 6 | 0.99 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 3 | 0.99 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 3 | 0.99 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 3 | 0.99 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 13 | 0.99 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 18 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 11 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 11 | 0.99 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 11 | 0.99 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 8 | 0.99 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 8 | 0.99 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 8 | 0.99 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 6 | 0.99 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 6 | 0.99 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 6 | 0.99 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 20 | 0.99 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 20 | 0.99 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 16 | 0.99 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 16 | 0.99 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 16 | 0.99 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 16 | 0.99 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 3 | 0.99 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 3 | 0.99 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 3 | 0.99 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 12 | 0.99 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 12 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 12 | 0.99 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 12 | 0.99 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 20 | 0.99 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 20 | 0.99 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 20 | 0.99 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 20 | 0.99 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 20 | 0.99 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 6 | 0.99 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 6 | 0.99 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 6 | 0.99 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 6 | 0.99 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 6 | 0.99 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 6 | 0.99 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 6 | 0.99 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 6 | 0.99 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG21 | 5 | 0.98 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG22 | 5 | 0.98 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG23 | 5 | 0.98 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG21 | 5 | 0.98 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG22 | 5 | 0.98 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG23 | 5 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 16 | 0.98 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 16 | 0.98 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 20 | 0.98 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 20 | 0.98 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 19 | 0.98 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 15 | 0.98 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 15 | 0.98 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 11 | 0.98 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 11 | 0.98 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 18 | 0.98 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 18 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 16 | 0.98 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 16 | 0.98 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 16 | 0.98 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 20 | 0.98 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 18 | 0.98 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 14 | 0.98 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 14 | 0.98 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 14 | 0.98 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 17 | 0.98 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 17 | 0.98 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 1 | 0.98 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 1 | 0.98 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 7 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 6 | 0.98 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 6 | 0.98 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 19 | 0.98 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 19 | 0.98 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 19 | 0.98 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 13 | 0.98 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 7 | 0.98 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 7 | 0.98 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 7 | 0.98 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 3 | 0.98 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 8 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 1 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 1 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 1 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 9 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 9 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 9 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 13 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 13 | 0.98 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 13 | 0.98 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 8 | 0.98 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 11 | 0.98 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 11 | 0.98 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 11 | 0.98 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 12 | 0.98 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 12 | 0.98 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 12 | 0.98 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 11 | 0.98 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 11 | 0.98 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 11 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 9 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 9 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 9 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 10 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 10 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 10 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 13 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 13 | 0.98 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 13 | 0.98 |
| (1,643) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 10 | 0.98 |
| (1,615) | 1:94:A:ALA:H | 1:97:A:GLN:HG2 | 20 | 0.98 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 4 | 0.98 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 4 | 0.98 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 4 | 0.98 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 4 | 0.98 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 4 | 0.98 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 4 | 0.98 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 14 | 0.98 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 17 | 0.98 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 17 | 0.98 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 17 | 0.98 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 17 | 0.98 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 17 | 0.98 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 17 | 0.98 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 9 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 9 | 0.98 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 9 | 0.98 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 9 | 0.97 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 9 | 0.97 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 5 | 0.97 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 5 | 0.97 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 5 | 0.97 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 5 | 0.97 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 5 | 0.97 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 5 | 0.97 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 20 | 0.97 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 20 | 0.97 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 19 | 0.97 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 2 | 0.97 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 2 | 0.97 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 7 | 0.97 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 11 | 0.97 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 11 | 0.97 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 5 | 0.97 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 5 | 0.97 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 5 | 0.97 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 18 | 0.97 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 13 | 0.97 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 5 | 0.97 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 5 | 0.97 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 5 | 0.97 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 5 | 0.97 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 5 | 0.97 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 5 | 0.97 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 1 | 0.97 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 20 | 0.97 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 8 | 0.97 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 5 | 0.97 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 5 | 0.97 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 5 | 0.97 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 17 | 0.97 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 19 | 0.97 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB1 | 5 | 0.97 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB2 | 5 | 0.97 |
| (1,1781) | 1:180:A:ILE:HA | 1:213:A:ALA:HB3 | 5 | 0.97 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 8 | 0.97 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 8 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 9 | 0.97 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 9 | 0.97 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 9 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 16 | 0.97 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 16 | 0.97 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 3 | 0.97 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 3 | 0.97 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 3 | 0.97 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 6 | 0.97 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 7 | 0.97 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 7 | 0.97 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 7 | 0.97 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 13 | 0.97 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 5 | 0.97 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 20 | 0.97 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 16 | 0.97 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 9 | 0.97 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 9 | 0.97 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 9 | 0.97 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 19 | 0.97 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 19 | 0.97 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 19 | 0.97 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 9 | 0.97 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 1 | 0.97 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 10 | 0.97 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 10 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 10 | 0.97 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 10 | 0.97 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 10 | 0.97 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 10 | 0.97 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 12 | 0.97 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 12 | 0.97 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 12 | 0.97 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 12 | 0.97 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 12 | 0.97 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 12 | 0.97 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 6 | 0.97 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 4 | 0.97 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 4 | 0.97 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 4 | 0.97 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 7 | 0.97 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 9 | 0.96 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 9 | 0.96 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 9 | 0.96 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 9 | 0.96 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 9 | 0.96 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 9 | 0.96 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 7 | 0.96 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 7 | 0.96 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 7 | 0.96 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 7 | 0.96 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 18 | 0.96 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 18 | 0.96 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 1 | 0.96 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 16 | 0.96 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 16 | 0.96 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 16 | 0.96 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 16 | 0.96 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 16 | 0.96 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 16 | 0.96 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 16 | 0.96 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 18 | 0.96 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 18 | 0.96 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 10 | 0.96 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 6 | 0.96 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 16 | 0.96 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 16 | 0.96 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 16 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 17 | 0.96 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 19 | 0.96 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 10 | 0.96 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 8 | 0.96 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 8 | 0.96 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 17 | 0.96 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 17 | 0.96 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 10 | 0.96 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 10 | 0.96 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 20 | 0.96 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 20 | 0.96 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 10 | 0.96 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 13 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 20 | 0.96 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 20 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 5 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 5 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 5 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 6 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 6 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 6 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 14 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 14 | 0.96 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 14 | 0.96 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 20 | 0.96 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 20 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 9 | 0.96 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 8 | 0.96 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 10 | 0.96 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 10 | 0.96 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 10 | 0.96 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 9 | 0.96 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 3 | 0.96 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 3 | 0.96 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 3 | 0.96 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 10 | 0.96 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 10 | 0.96 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 10 | 0.96 |
| (1,664) | 1:103:A:THR:HA | 1:128:A:LEU:H | 20 | 0.96 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB2 | 15 | 0.96 |
| (1,608) | 1:212:A:LYS:HD2 | 1:215:A:GLU:HB3 | 15 | 0.96 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB2 | 15 | 0.96 |
| (1,608) | 1:212:A:LYS:HD3 | 1:215:A:GLU:HB3 | 15 | 0.96 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 19 | 0.96 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 19 | 0.96 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 19 | 0.96 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 6 | 0.96 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 12 | 0.96 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 3 | 0.96 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 3 | 0.96 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 2 | 0.96 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 2 | 0.96 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 2 | 0.96 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 12 | 0.96 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 12 | 0.96 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 12 | 0.96 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 18 | 0.96 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 18 | 0.96 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 18 | 0.96 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 3 | 0.96 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 3 | 0.96 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 3 | 0.96 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 19 | 0.96 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 19 | 0.96 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 19 | 0.96 |
| (1,20) | 1:47:A:THR:HG21 | 1:50:A:LEU:HA | 3 | 0.96 |
| (1,20) | 1:47:A:THR:HG22 | 1:50:A:LEU:HA | 3 | 0.96 |
| (1,20) | 1:47:A:THR:HG23 | 1:50:A:LEU:HA | 3 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 20 | 0.96 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 19 | 0.96 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 5 | 0.95 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 5 | 0.95 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 13 | 0.95 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 13 | 0.95 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 20 | 0.95 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 20 | 0.95 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 20 | 0.95 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 20 | 0.95 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 16 | 0.95 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 16 | 0.95 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 20 | 0.95 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 20 | 0.95 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 20 | 0.95 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 7 | 0.95 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 20 | 0.95 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 20 | 0.95 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 8 | 0.95 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 8 | 0.95 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 7 | 0.95 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 20 | 0.95 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 9 | 0.95 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 9 | 0.95 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 9 | 0.95 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 9 | 0.95 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 9 | 0.95 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 9 | 0.95 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 5 | 0.95 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 17 | 0.95 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 4 | 0.95 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 7 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 17 | 0.95 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 13 | 0.95 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 13 | 0.95 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 13 | 0.95 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 16 | 0.95 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 16 | 0.95 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 20 | 0.95 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 20 | 0.95 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 2 | 0.95 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 2 | 0.95 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 2 | 0.95 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 7 | 0.95 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 14 | 0.95 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 15 | 0.95 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 7 | 0.95 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 7 | 0.95 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 7 | 0.95 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 7 | 0.95 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 7 | 0.95 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 7 | 0.95 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 18 | 0.95 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 6 | 0.95 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 6 | 0.95 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 6 | 0.95 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 1 | 0.95 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 3 | 0.95 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 9 | 0.95 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 8 | 0.95 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 8 | 0.95 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 8 | 0.95 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 8 | 0.95 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 19 | 0.95 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 19 | 0.95 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 19 | 0.95 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 19 | 0.95 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 19 | 0.95 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 19 | 0.95 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 12 | 0.95 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 4 | 0.95 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 4 | 0.95 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 2 | 0.95 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 2 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 2 | 0.95 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 6 | 0.95 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 6 | 0.95 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 6 | 0.95 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 6 | 0.95 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 6 | 0.95 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 6 | 0.95 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 8 | 0.95 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 14 | 0.95 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 11 | 0.95 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 9 | 0.95 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 9 | 0.95 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 9 | 0.94 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 9 | 0.94 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 17 | 0.94 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 17 | 0.94 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 7 | 0.94 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 7 | 0.94 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 7 | 0.94 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 7 | 0.94 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 7 | 0.94 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 7 | 0.94 |
| (1,3548) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG2 | 3 | 0.94 |
| (1,3548) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 3 | 0.94 |
| (1,3548) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG2 | 3 | 0.94 |
| (1,3548) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 3 | 0.94 |
| (1,3548) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG2 | 3 | 0.94 |
| (1,3548) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 3 | 0.94 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 3 | 0.94 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 3 | 0.94 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 13 | 0.94 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 13 | 0.94 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 13 | 0.94 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 2 | 0.94 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 18 | 0.94 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 13 | 0.94 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 12 | 0.94 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 7 | 0.94 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 8 | 0.94 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 13 | 0.94 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 10 | 0.94 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 2 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 2 | 0.94 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 2 | 0.94 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 4 | 0.94 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 19 | 0.94 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 19 | 0.94 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 1 | 0.94 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 9 | 0.94 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 2 | 0.94 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 2 | 0.94 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 2 | 0.94 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 1 | 0.94 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 1 | 0.94 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 9 | 0.94 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 9 | 0.94 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 14 | 0.94 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 14 | 0.94 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 1 | 0.94 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 1 | 0.94 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 8 | 0.94 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 11 | 0.94 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 11 | 0.94 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 6 | 0.94 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 5 | 0.94 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 5 | 0.94 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 5 | 0.94 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 15 | 0.94 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 15 | 0.94 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 15 | 0.94 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 8 | 0.94 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 8 | 0.94 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 8 | 0.94 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 18 | 0.94 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 18 | 0.94 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 2 | 0.94 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 2 | 0.94 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 14 | 0.94 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 14 | 0.94 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 14 | 0.94 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 1 | 0.94 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 7 | 0.94 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 7 | 0.94 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 7 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 8 | 0.94 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 6 | 0.94 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 6 | 0.94 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 5 | 0.94 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 16 | 0.94 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 13 | 0.94 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 13 | 0.94 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 6 | 0.94 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 6 | 0.94 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 6 | 0.94 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 12 | 0.94 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 12 | 0.94 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 12 | 0.94 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 14 | 0.94 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 14 | 0.94 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 14 | 0.94 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 6 | 0.94 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 10 | 0.93 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 10 | 0.93 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 10 | 0.93 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 10 | 0.93 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 10 | 0.93 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 10 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 12 | 0.93 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 12 | 0.93 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 17 | 0.93 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 17 | 0.93 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 17 | 0.93 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 17 | 0.93 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 17 | 0.93 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 17 | 0.93 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 5 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 5 | 0.93 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 2 | 0.93 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 7 | 0.93 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 7 | 0.93 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 12 | 0.93 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 3 | 0.93 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 11 | 0.93 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 9 | 0.93 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 7 | 0.93 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 15 | 0.93 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 14 | 0.93 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 14 | 0.93 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 3 | 0.93 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 3 | 0.93 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 3 | 0.93 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 5 | 0.93 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 5 | 0.93 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 10 | 0.93 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 10 | 0.93 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 17 | 0.93 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 9 | 0.93 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 9 | 0.93 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 14 | 0.93 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 14 | 0.93 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 14 | 0.93 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 18 | 0.93 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 12 | 0.93 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 12 | 0.93 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 12 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 17 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 17 | 0.93 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 17 | 0.93 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 3 | 0.93 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 14 | 0.93 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 14 | 0.93 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 14 | 0.93 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 18 | 0.93 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 18 | 0.93 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 18 | 0.93 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 4 | 0.93 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 4 | 0.93 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 4 | 0.93 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 1 | 0.93 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 1 | 0.93 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 8 | 0.93 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 8 | 0.93 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 14 | 0.93 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 13 | 0.93 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 13 | 0.93 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 13 | 0.93 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 6 | 0.93 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 6 | 0.93 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 6 | 0.93 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 8 | 0.93 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 8 | 0.93 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 8 | 0.93 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 10 | 0.93 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 8 | 0.92 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 8 | 0.92 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 8 | 0.92 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 8 | 0.92 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 5 | 0.92 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 5 | 0.92 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 5 | 0.92 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 5 | 0.92 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 5 | 0.92 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 5 | 0.92 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG21 | 16 | 0.92 |
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG22 | 16 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3764) | 1:113:A:ASP:HB2 | 1:117:A:VAL:HG23 | 16 | 0.92 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG21 | 16 | 0.92 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG22 | 16 | 0.92 |
| (1,3764) | 1:113:A:ASP:HB3 | 1:117:A:VAL:HG23 | 16 | 0.92 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 16 | 0.92 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 16 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 16 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 16 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 16 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 16 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 16 | 0.92 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 16 | 0.92 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 14 | 0.92 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 14 | 0.92 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 8 | 0.92 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 8 | 0.92 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 8 | 0.92 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 8 | 0.92 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 2 | 0.92 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 2 | 0.92 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 5 | 0.92 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 5 | 0.92 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 8 | 0.92 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 8 | 0.92 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 17 | 0.92 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 17 | 0.92 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 19 | 0.92 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 19 | 0.92 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 3 | 0.92 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 3 | 0.92 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 12 | 0.92 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 12 | 0.92 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 16 | 0.92 |
| (1,3074) | 1:167:A:ASP:H | 1:196:A:ASN:HD22 | 19 | 0.92 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 6 | 0.92 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 1 | 0.92 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 3 | 0.92 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 18 | 0.92 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 17 | 0.92 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 17 | 0.92 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 17 | 0.92 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 18 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 18 | 0.92 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 18 | 0.92 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 4 | 0.92 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 17 | 0.92 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 17 | 0.92 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 17 | 0.92 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 14 | 0.92 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 14 | 0.92 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 14 | 0.92 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 3 | 0.92 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 3 | 0.92 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 5 | 0.92 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 5 | 0.92 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 16 | 0.92 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 7 | 0.92 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 7 | 0.92 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 7 | 0.92 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 6 | 0.92 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 6 | 0.92 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 6 | 0.92 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 14 | 0.92 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 6 | 0.92 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 6 | 0.92 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 6 | 0.92 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 14 | 0.92 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 20 | 0.92 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 20 | 0.92 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 14 | 0.92 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 14 | 0.92 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 14 | 0.92 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 10 | 0.92 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 10 | 0.92 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 13 | 0.92 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 13 | 0.92 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 5 | 0.92 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 5 | 0.92 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 5 | 0.92 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 19 | 0.92 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 20 | 0.92 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 17 | 0.92 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 17 | 0.92 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 17 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 18 | 0.92 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 18 | 0.92 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 18 | 0.92 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 20 | 0.92 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 20 | 0.92 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 6 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 6 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 6 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 6 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 6 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 6 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 9 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 9 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 9 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 9 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 9 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 9 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 11 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 11 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 11 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 11 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 11 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 11 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 18 | 0.91 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 18 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 18 | 0.91 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 18 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 18 | 0.91 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 18 | 0.91 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 10 | 0.91 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 9 | 0.91 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 9 | 0.91 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 18 | 0.91 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 18 | 0.91 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 2 | 0.91 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 13 | 0.91 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 15 | 0.91 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 20 | 0.91 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 8 | 0.91 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 3 | 0.91 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 1 | 0.91 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 6 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 11 | 0.91 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 11 | 0.91 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 11 | 0.91 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 11 | 0.91 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 11 | 0.91 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 13 | 0.91 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 13 | 0.91 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 13 | 0.91 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 16 | 0.91 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 6 | 0.91 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 6 | 0.91 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 13 | 0.91 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 13 | 0.91 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 14 | 0.91 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 14 | 0.91 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 11 | 0.91 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 11 | 0.91 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 11 | 0.91 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 16 | 0.91 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 16 | 0.91 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 16 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 4 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 13 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 13 | 0.91 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 13 | 0.91 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 15 | 0.91 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 4 | 0.91 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 4 | 0.91 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 4 | 0.91 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 13 | 0.91 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 13 | 0.91 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 13 | 0.91 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 16 | 0.91 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 16 | 0.91 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 16 | 0.91 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 19 | 0.91 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 8 | 0.91 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 17 | 0.91 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 9 | 0.91 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 9 | 0.91 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 9 | 0.91 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG11 | 5 | 0.91 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG12 | 5 | 0.91 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG13 | 5 | 0.91 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG11 | 5 | 0.91 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG12 | 5 | 0.91 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG13 | 5 | 0.91 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 18 | 0.91 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 11 | 0.91 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 8 | 0.91 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 3 | 0.91 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 16 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 16 | 0.91 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 16 | 0.91 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 15 | 0.9 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 15 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 2 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 2 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 2 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 2 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 2 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 2 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 4 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 4 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 4 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 4 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 4 | 0.9 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 4 | 0.9 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG21 | 13 | 0.9 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG22 | 13 | 0.9 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG23 | 13 | 0.9 |
| (1,3386) | 2:8:B:ILE:HD11 | 2:9:B:ILE:H | 8 | 0.9 |
| (1,3386) | 2:8:B:ILE:HD12 | 2:9:B:ILE:H | 8 | 0.9 |
| (1,3386) | 2:8:B:ILE:HD13 | 2:9:B:ILE:H | 8 | 0.9 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 5 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 2 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 2 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 13 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 13 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 16 | 0.9 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 16 | 0.9 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 13 | 0.9 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 13 | 0.9 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 2 | 0.9 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 15 | 0.9 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 16 | 0.9 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 18 | 0.9 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 6 | 0.9 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 17 | 0.9 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 19 | 0.9 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 19 | 0.9 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 7 | 0.9 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 9 | 0.9 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 7 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 5 | 0.9 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 5 | 0.9 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 5 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 4 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 4 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 4 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 11 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 11 | 0.9 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 11 | 0.9 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 12 | 0.9 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 12 | 0.9 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 2 | 0.9 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 2 | 0.9 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 4 | 0.9 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 4 | 0.9 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 4 | 0.9 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 4 | 0.9 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 4 | 0.9 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 17 | 0.9 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 17 | 0.9 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 17 | 0.9 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 7 | 0.9 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 7 | 0.9 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 7 | 0.9 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 7 | 0.9 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 7 | 0.9 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 7 | 0.9 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 19 | 0.9 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 19 | 0.9 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 19 | 0.9 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 3 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 8 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 8 | 0.9 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 8 | 0.9 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 20 | 0.9 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 20 | 0.9 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 20 | 0.9 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 14 | 0.9 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 20 | 0.9 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 20 | 0.9 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 20 | 0.9 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 2 | 0.9 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 7 | 0.9 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 7 | 0.9 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 7 | 0.9 |
| (1,1090) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB2 | 5 | 0.9 |
| (1,1090) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB2 | 5 | 0.9 |
| (1,1090) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB2 | 5 | 0.9 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 14 | 0.9 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 11 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 9 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 9 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 9 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 11 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 11 | 0.9 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 11 | 0.9 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 15 | 0.9 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 20 | 0.9 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 20 | 0.9 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 20 | 0.9 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 3 | 0.89 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 3 | 0.89 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 2 | 0.89 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 2 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 6 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 6 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 6 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 6 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 6 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 6 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 12 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 12 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 12 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 12 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 12 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 12 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 20 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 20 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 20 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 20 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 20 | 0.89 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 20 | 0.89 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 19 | 0.89 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 19 | 0.89 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 19 | 0.89 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 19 | 0.89 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 19 | 0.89 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 19 | 0.89 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 7 | 0.89 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 7 | 0.89 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 7 | 0.89 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 16 | 0.89 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 19 | 0.89 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 19 | 0.89 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 19 | 0.89 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 19 | 0.89 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 1 | 0.89 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 1 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 6 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 6 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 6 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 15 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 15 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 15 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 17 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 17 | 0.89 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 17 | 0.89 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 3 | 0.89 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 4 | 0.89 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 4 | 0.89 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 7 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 3 | 0.89 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 6 | 0.89 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 7 | 0.89 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 20 | 0.89 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 18 | 0.89 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 19 | 0.89 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 12 | 0.89 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 14 | 0.89 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 4 | 0.89 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 4 | 0.89 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 4 | 0.89 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 8 | 0.89 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB2 | 15 | 0.89 |
| (1,1969) | 1:213:A:ALA:HA | 1:215:A:GLU:HB3 | 15 | 0.89 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 6 | 0.89 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 6 | 0.89 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 7 | 0.89 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 7 | 0.89 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 5 | 0.89 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 5 | 0.89 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 5 | 0.89 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 19 | 0.89 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 19 | 0.89 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 19 | 0.89 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 10 | 0.89 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 10 | 0.89 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 10 | 0.89 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 10 | 0.89 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 10 | 0.89 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 10 | 0.89 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 15 | 0.89 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 15 | 0.89 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 10 | 0.89 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 6 | 0.89 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 12 | 0.89 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 12 | 0.89 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 12 | 0.89 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 5 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 2 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 2 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 14 | 0.89 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 14 | 0.89 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 9 | 0.89 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 9 | 0.89 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 9 | 0.89 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 11 | 0.89 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 11 | 0.89 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 11 | 0.89 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 5 | 0.89 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 2 | 0.89 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 5 | 0.89 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 5 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 5 | 0.89 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 19 | 0.89 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 6 | 0.89 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 6 | 0.89 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 6 | 0.89 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 1 | 0.89 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 1 | 0.89 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 1 | 0.89 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 20 | 0.89 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 20 | 0.89 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 20 | 0.89 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 20 | 0.89 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 20 | 0.89 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 20 | 0.89 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 20 | 0.89 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 1 | 0.89 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 12 | 0.89 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 12 | 0.89 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 9 | 0.89 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 9 | 0.89 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 14 | 0.89 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 14 | 0.89 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 14 | 0.89 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 9 | 0.89 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 9 | 0.89 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 9 | 0.89 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 13 | 0.89 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 13 | 0.89 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 13 | 0.89 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 4 | 0.89 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 4 | 0.89 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 4 | 0.89 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 4 | 0.89 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 4 | 0.89 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 4 | 0.89 |
| (1,14) | 1:47:A:THR:HB | 1:49:A:ASP:H | 11 | 0.89 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 10 | 0.88 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 10 | 0.88 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD21 | 19 | 0.88 |
| (1,3856) | 1:147:A:GLY:H | 1:175:A:ASN:HD22 | 19 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 18 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 18 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 18 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 18 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 18 | 0.88 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 18 | 0.88 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 11 | 0.88 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 11 | 0.88 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 11 | 0.88 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 11 | 0.88 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 15 | 0.88 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 15 | 0.88 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 4 | 0.88 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 4 | 0.88 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 4 | 0.88 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 1 | 0.88 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 1 | 0.88 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 13 | 0.88 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 13 | 0.88 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 14 | 0.88 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 14 | 0.88 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 2 | 0.88 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 2 | 0.88 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 16 | 0.88 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 16 | 0.88 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 6 | 0.88 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 10 | 0.88 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 15 | 0.88 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 19 | 0.88 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 20 | 0.88 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 20 | 0.88 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 20 | 0.88 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 6 | 0.88 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 4 | 0.88 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 4 | 0.88 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 18 | 0.88 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 18 | 0.88 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 18 | 0.88 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 5 | 0.88 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 7 | 0.88 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 8 | 0.88 |
| (1,1733) | 1:196:A:ASN:HB3 | 1:225:A:LYS:HB2 | 15 | 0.88 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 7 | 0.88 |
| (1,1727) | 1:168:A:ALA:H | 1:196:A:ASN:HB3 | 19 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 7 | 0.88 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 7 | 0.88 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 7 | 0.88 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 13 | 0.88 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 13 | 0.88 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 13 | 0.88 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 13 | 0.88 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 13 | 0.88 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 13 | 0.88 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 11 | 0.88 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 13 | 0.88 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 13 | 0.88 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 13 | 0.88 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 10 | 0.88 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 13 | 0.88 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 6 | 0.88 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 6 | 0.88 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 6 | 0.88 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 8 | 0.88 |
| (1,613) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG2 | 4 | 0.88 |
| (1,613) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG2 | 4 | 0.88 |
| (1,613) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG2 | 4 | 0.88 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 11 | 0.88 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 11 | 0.88 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 14 | 0.88 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 14 | 0.88 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 14 | 0.88 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 7 | 0.88 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 19 | 0.88 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 19 | 0.88 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 19 | 0.88 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 19 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 19 | 0.88 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 19 | 0.88 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 1 | 0.88 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 1 | 0.88 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 1 | 0.88 |
| (1,32) | 1:153:A:VAL:HG11 | 1:166:A:ASP:HB3 | 16 | 0.88 |
| (1,32) | 1:153:A:VAL:HG12 | 1:166:A:ASP:HB3 | 16 | 0.88 |
| (1,32) | 1:153:A:VAL:HG13 | 1:166:A:ASP:HB3 | 16 | 0.88 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 6 | 0.87 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 6 | 0.87 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 1 | 0.87 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 1 | 0.87 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 1 | 0.87 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 1 | 0.87 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 1 | 0.87 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 1 | 0.87 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 11 | 0.87 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 11 | 0.87 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 17 | 0.87 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 17 | 0.87 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 7 | 0.87 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 7 | 0.87 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 15 | 0.87 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 15 | 0.87 |
| (1,3387) | 2:8:B:ILE:HD11 | 2:21:B:MET:H | 8 | 0.87 |
| (1,3387) | 2:8:B:ILE:HD12 | 2:21:B:MET:H | 8 | 0.87 |
| (1,3387) | 2:8:B:ILE:HD13 | 2:21:B:MET:H | 8 | 0.87 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 6 | 0.87 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 6 | 0.87 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 6 | 0.87 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 18 | 0.87 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 18 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 18 | 0.87 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 13 | 0.87 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 7 | 0.87 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 7 | 0.87 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 13 | 0.87 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 16 | 0.87 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 2 | 0.87 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 15 | 0.87 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 15 | 0.87 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 15 | 0.87 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 15 | 0.87 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 15 | 0.87 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 15 | 0.87 |
| (1,2645) | 1:148:A:SER:H | 1:179:A:LEU:HB3 | 19 | 0.87 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 3 | 0.87 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 10 | 0.87 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 8 | 0.87 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 15 | 0.87 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 15 | 0.87 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 15 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 2 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 2 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 2 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 6 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 6 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 6 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 11 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 11 | 0.87 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 11 | 0.87 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 10 | 0.87 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 10 | 0.87 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 10 | 0.87 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 16 | 0.87 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 16 | 0.87 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 8 | 0.87 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 8 | 0.87 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 8 | 0.87 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 8 | 0.87 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 8 | 0.87 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 8 | 0.87 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 9 | 0.87 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 9 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 9 | 0.87 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 2 | 0.87 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 2 | 0.87 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 2 | 0.87 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 2 | 0.87 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 2 | 0.87 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 2 | 0.87 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 9 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 1 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 7 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 7 | 0.87 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 7 | 0.87 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 17 | 0.87 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 17 | 0.87 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 17 | 0.87 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 15 | 0.87 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 15 | 0.87 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 15 | 0.87 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 1 | 0.87 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 4 | 0.87 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 4 | 0.87 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 4 | 0.87 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 16 | 0.87 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 2 | 0.87 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 2 | 0.87 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 2 | 0.87 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 2 | 0.87 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 2 | 0.87 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 2 | 0.87 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 1 | 0.87 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 15 | 0.87 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 14 | 0.87 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 19 | 0.87 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 10 | 0.87 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 10 | 0.87 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 4 | 0.87 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 5 | 0.87 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 5 | 0.87 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 5 | 0.87 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 1 | 0.87 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 1 | 0.87 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 1 | 0.87 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 1 | 0.87 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 1 | 0.87 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 1 | 0.87 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD21 | 3 | 0.87 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD22 | 3 | 0.87 |
| (1,10) | 1:47:A:THR:HB | 1:50:A:LEU:HD23 | 3 | 0.87 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 3 | 0.87 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 3 | 0.87 |
| (1,3843) | 1:137:A:ASP:H | 1:152:A:LYS:HE2 | 2 | 0.86 |
| (1,3843) | 1:137:A:ASP:H | 1:152:A:LYS:HE3 | 2 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 9 | 0.86 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 9 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 7 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 7 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 7 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 7 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 7 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 7 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 15 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 15 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 15 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 15 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 15 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 15 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 19 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 19 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 19 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 19 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 19 | 0.86 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 19 | 0.86 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 3 | 0.86 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 3 | 0.86 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 12 | 0.86 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 12 | 0.86 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 12 | 0.86 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 4 | 0.86 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 4 | 0.86 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 4 | 0.86 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 4 | 0.86 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 4 | 0.86 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 4 | 0.86 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 4 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 5 | 0.86 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 5 | 0.86 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 20 | 0.86 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 20 | 0.86 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 11 | 0.86 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 11 | 0.86 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 2 | 0.86 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 18 | 0.86 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 18 | 0.86 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 18 | 0.86 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 18 | 0.86 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 18 | 0.86 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 18 | 0.86 |
| (1,2575) | 1:135:A:PHE:HB3 | 1:138:A:ALA:H | 11 | 0.86 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 1 | 0.86 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 1 | 0.86 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 1 | 0.86 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 7 | 0.86 |
| (1,2127) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB2 | 5 | 0.86 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 20 | 0.86 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 2 | 0.86 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 17 | 0.86 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 17 | 0.86 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 17 | 0.86 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 17 | 0.86 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 17 | 0.86 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 17 | 0.86 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 20 | 0.86 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 20 | 0.86 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 20 | 0.86 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 10 | 0.86 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 10 | 0.86 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 10 | 0.86 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 3 | 0.86 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 3 | 0.86 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 3 | 0.86 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 12 | 0.86 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 12 | 0.86 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 12 | 0.86 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 9 | 0.86 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 15 | 0.86 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 16 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 2 | 0.86 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 2 | 0.86 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 2 | 0.86 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 12 | 0.86 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 12 | 0.86 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 12 | 0.86 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 18 | 0.86 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 18 | 0.86 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 18 | 0.86 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 18 | 0.86 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 18 | 0.86 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 18 | 0.86 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 12 | 0.86 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 12 | 0.86 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 12 | 0.86 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 10 | 0.86 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 5 | 0.86 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 19 | 0.86 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 17 | 0.86 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 17 | 0.86 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 13 | 0.86 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 10 | 0.86 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 10 | 0.86 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 10 | 0.86 |
| (1,782) | 1:80:A:SER:HB2 | 1:114:A:ASP:HB3 | 2 | 0.86 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 8 | 0.86 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 1 | 0.86 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 2 | 0.86 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 7 | 0.86 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 13 | 0.86 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 13 | 0.86 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 13 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 2 | 0.86 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 2 | 0.86 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 2 | 0.86 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 20 | 0.86 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 11 | 0.86 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 7 | 0.86 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 7 | 0.86 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 7 | 0.86 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 7 | 0.86 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 7 | 0.86 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 7 | 0.86 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 18 | 0.86 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 18 | 0.86 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 18 | 0.86 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 13 | 0.86 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 1 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 3 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 11 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 11 | 0.85 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 11 | 0.85 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 13 | 0.85 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 13 | 0.85 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 13 | 0.85 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 13 | 0.85 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 16 | 0.85 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 16 | 0.85 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 16 | 0.85 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 16 | 0.85 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 12 | 0.85 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 12 | 0.85 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 9 | 0.85 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 15 | 0.85 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 15 | 0.85 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 4 | 0.85 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 4 | 0.85 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 4 | 0.85 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 4 | 0.85 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 4 | 0.85 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 4 | 0.85 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 10 | 0.85 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 18 | 0.85 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 17 | 0.85 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 11 | 0.85 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 11 | 0.85 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 11 | 0.85 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 19 | 0.85 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 19 | 0.85 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 19 | 0.85 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 19 | 0.85 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 19 | 0.85 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 5 | 0.85 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 5 | 0.85 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 5 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 10 | 0.85 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 10 | 0.85 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 10 | 0.85 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 16 | 0.85 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 16 | 0.85 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 16 | 0.85 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 16 | 0.85 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 16 | 0.85 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 16 | 0.85 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 20 | 0.85 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 20 | 0.85 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 20 | 0.85 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 20 | 0.85 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 20 | 0.85 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 20 | 0.85 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 7 | 0.85 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 7 | 0.85 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 6 | 0.85 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 6 | 0.85 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 6 | 0.85 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 17 | 0.85 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 17 | 0.85 |
| (1,1544) | 1:184:A:ILE:HA | 1:187:A:MET:HG3 | 9 | 0.85 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 19 | 0.85 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 7 | 0.85 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 7 | 0.85 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 7 | 0.85 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 13 | 0.85 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 15 | 0.85 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 12 | 0.85 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 6 | 0.85 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 2 | 0.85 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 2 | 0.85 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 15 | 0.85 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 18 | 0.85 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 18 | 0.85 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 18 | 0.85 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 1 | 0.85 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 1 | 0.85 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 1 | 0.85 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 20 | 0.85 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 20 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 20 | 0.85 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 10 | 0.85 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 20 | 0.85 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 18 | 0.84 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 18 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 3 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 3 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 3 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 3 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 3 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 3 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 14 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 14 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 14 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 14 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 14 | 0.84 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 14 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 7 | 0.84 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 7 | 0.84 |
| (1,3623) | 1:81:A:ARG:HD2 | 1:83:A:GLN:HG2 | 15 | 0.84 |
| (1,3623) | 1:81:A:ARG:HD3 | 1:83:A:GLN:HG2 | 15 | 0.84 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 2 | 0.84 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 2 | 0.84 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 10 | 0.84 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 10 | 0.84 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 2 | 0.84 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 2 | 0.84 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 2 | 0.84 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 2 | 0.84 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 2 | 0.84 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 2 | 0.84 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 8 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 8 | 0.84 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 8 | 0.84 |
| (1,3104) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HD1 | 4 | 0.84 |
| (1,3104) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HD2 | 4 | 0.84 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 16 | 0.84 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 11 | 0.84 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD11 | 19 | 0.84 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD12 | 19 | 0.84 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD13 | 19 | 0.84 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 1 | 0.84 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 14 | 0.84 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 12 | 0.84 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 12 | 0.84 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 12 | 0.84 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 18 | 0.84 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 18 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 1 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 1 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 1 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 1 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 1 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 1 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 13 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 13 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 13 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 13 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 13 | 0.84 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 13 | 0.84 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 13 | 0.84 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 18 | 0.84 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 18 | 0.84 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 18 | 0.84 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 12 | 0.84 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 16 | 0.84 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 9 | 0.84 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 9 | 0.84 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 9 | 0.84 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 18 | 0.84 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 18 | 0.84 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 18 | 0.84 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 16 | 0.84 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 16 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 3 | 0.84 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 3 | 0.84 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 3 | 0.84 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 19 | 0.84 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 20 | 0.84 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 14 | 0.84 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 10 | 0.84 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 10 | 0.84 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 10 | 0.84 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 14 | 0.84 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 14 | 0.84 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 14 | 0.84 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 14 | 0.84 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 14 | 0.84 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 14 | 0.84 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 4 | 0.84 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG21 | 12 | 0.84 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG22 | 12 | 0.84 |
| (1,315) | 1:60:A:LYS:HD2 | 1:70:A:THR:HG23 | 12 | 0.84 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG21 | 12 | 0.84 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG22 | 12 | 0.84 |
| (1,315) | 1:60:A:LYS:HD3 | 1:70:A:THR:HG23 | 12 | 0.84 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 4 | 0.84 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 4 | 0.84 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 4 | 0.84 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 8 | 0.84 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 8 | 0.84 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 8 | 0.84 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 8 | 0.84 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 8 | 0.84 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 7 | 0.84 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 17 | 0.83 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 17 | 0.83 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 5 | 0.83 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 5 | 0.83 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 18 | 0.83 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 18 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 8 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 8 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 8 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 8 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 8 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 8 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG11 | 11 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG12 | 11 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG13 | 11 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG21 | 11 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG22 | 11 | 0.83 |
| (1,3730) | 1:109:A:ASN:HD21 | 1:110:A:VAL:HG23 | 11 | 0.83 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 13 | 0.83 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 13 | 0.83 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 17 | 0.83 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 17 | 0.83 |
| (1,3347) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB2 | 15 | 0.83 |
| (1,3347) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB2 | 15 | 0.83 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 5 | 0.83 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 4 | 0.83 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 4 | 0.83 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 4 | 0.83 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 18 | 0.83 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 7 | 0.83 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 7 | 0.83 |
| (1,3204) | 1:88:A:GLN:HB3 | 1:90:A:HIS:HE1 | 8 | 0.83 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 7 | 0.83 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 7 | 0.83 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 2 | 0.83 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 8 | 0.83 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 15 | 0.83 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 15 | 0.83 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 15 | 0.83 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 14 | 0.83 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 13 | 0.83 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 13 | 0.83 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 8 | 0.83 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 18 | 0.83 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 18 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 4 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 4 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 4 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 14 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 14 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 14 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 16 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 16 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 16 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 18 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 18 | 0.83 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 18 | 0.83 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 6 | 0.83 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 15 | 0.83 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 20 | 0.83 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 1 | 0.83 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 6 | 0.83 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 16 | 0.83 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 1 | 0.83 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 1 | 0.83 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 1 | 0.83 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 1 | 0.83 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 1 | 0.83 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 1 | 0.83 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 5 | 0.83 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 5 | 0.83 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 5 | 0.83 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 5 | 0.83 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 5 | 0.83 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 5 | 0.83 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 5 | 0.83 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 5 | 0.83 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 5 | 0.83 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 19 | 0.83 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 19 | 0.83 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 19 | 0.83 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 1 | 0.83 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 1 | 0.83 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 1 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 10 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 10 | 0.83 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 10 | 0.83 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 20 | 0.83 |
| (1,1413) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB3 | 7 | 0.83 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 17 | 0.83 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 17 | 0.83 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 17 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 6 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 6 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 6 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 6 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 6 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 6 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 13 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 13 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 13 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 13 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 13 | 0.83 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 13 | 0.83 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 4 | 0.83 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 4 | 0.83 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 4 | 0.83 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 4 | 0.83 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 4 | 0.83 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 4 | 0.83 |
| (1,1057) | 1:139:A:SER:HB3 | 1:151:A:ALA:H | 12 | 0.83 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 3 | 0.83 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 11 | 0.83 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 8 | 0.83 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 12 | 0.83 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 6 | 0.83 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 6 | 0.83 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 6 | 0.83 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 15 | 0.83 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 20 | 0.83 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 8 | 0.83 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 8 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 14 | 0.83 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 14 | 0.83 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 14 | 0.83 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 14 | 0.83 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 14 | 0.83 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 2 | 0.83 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 2 | 0.83 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 2 | 0.83 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 12 | 0.83 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 18 | 0.83 |
| (1,190) | 1:59:A:ALA:HA | 2:12:B:ASN:HD22 | 10 | 0.83 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 8 | 0.83 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 8 | 0.83 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 8 | 0.83 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 8 | 0.83 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 8 | 0.83 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 8 | 0.83 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 10 | 0.83 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 9 | 0.82 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 9 | 0.82 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 18 | 0.82 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 18 | 0.82 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 18 | 0.82 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 18 | 0.82 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 18 | 0.82 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 18 | 0.82 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 8 | 0.82 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 8 | 0.82 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 8 | 0.82 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 8 | 0.82 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 8 | 0.82 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 8 | 0.82 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 14 | 0.82 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 14 | 0.82 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 14 | 0.82 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 14 | 0.82 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 14 | 0.82 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 14 | 0.82 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 12 | 0.82 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 12 | 0.82 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 5 | 0.82 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 5 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 12 | 0.82 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 12 | 0.82 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 12 | 0.82 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 1 | 0.82 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 1 | 0.82 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 1 | 0.82 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 13 | 0.82 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 13 | 0.82 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 13 | 0.82 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 13 | 0.82 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 8 | 0.82 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 8 | 0.82 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 12 | 0.82 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 12 | 0.82 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 7 | 0.82 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 7 | 0.82 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 7 | 0.82 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 11 | 0.82 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 11 | 0.82 |
| (1,3079) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 5 | 0.82 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 20 | 0.82 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 11 | 0.82 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 6 | 0.82 |
| (1,2375) | 1:92:A:LYS:HG2 | 1:93:A:GLU:H | 4 | 0.82 |
| (1,2375) | 1:92:A:LYS:HG3 | 1:93:A:GLU:H | 4 | 0.82 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD11 | 3 | 0.82 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD12 | 3 | 0.82 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD13 | 3 | 0.82 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 3 | 0.82 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 3 | 0.82 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 8 | 0.82 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 12 | 0.82 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 12 | 0.82 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 12 | 0.82 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 12 | 0.82 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 12 | 0.82 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 12 | 0.82 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 6 | 0.82 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 6 | 0.82 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 6 | 0.82 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 15 | 0.82 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 15 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 15 | 0.82 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 11 | 0.82 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 11 | 0.82 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 11 | 0.82 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 11 | 0.82 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 11 | 0.82 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 11 | 0.82 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 14 | 0.82 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 14 | 0.82 |
| (1,1412) | 1:174:A:GLU:HG2 | 1:177:A:GLU:HB3 | 1 | 0.82 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 17 | 0.82 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 17 | 0.82 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 17 | 0.82 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 17 | 0.82 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 17 | 0.82 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 17 | 0.82 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 20 | 0.82 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 2 | 0.82 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 2 | 0.82 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 2 | 0.82 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 11 | 0.82 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 11 | 0.82 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 11 | 0.82 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 11 | 0.82 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 11 | 0.82 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 11 | 0.82 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 20 | 0.82 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 20 | 0.82 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 20 | 0.82 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 19 | 0.82 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 19 | 0.82 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 19 | 0.82 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 18 | 0.82 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 16 | 0.82 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 16 | 0.82 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 8 | 0.82 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 5 | 0.82 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 5 | 0.82 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 5 | 0.82 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 6 | 0.82 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 19 | 0.82 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 3 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 1 | 0.82 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 1 | 0.82 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 1 | 0.82 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 3 | 0.81 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 3 | 0.81 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 3 | 0.81 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 3 | 0.81 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 3 | 0.81 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 3 | 0.81 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 14 | 0.81 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 14 | 0.81 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 14 | 0.81 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 14 | 0.81 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 14 | 0.81 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 14 | 0.81 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 10 | 0.81 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 10 | 0.81 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 10 | 0.81 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 15 | 0.81 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 4 | 0.81 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 4 | 0.81 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 13 | 0.81 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 15 | 0.81 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 13 | 0.81 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 8 | 0.81 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 16 | 0.81 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 10 | 0.81 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 18 | 0.81 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 12 | 0.81 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 1 | 0.81 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 12 | 0.81 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 14 | 0.81 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 14 | 0.81 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 14 | 0.81 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 9 | 0.81 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 9 | 0.81 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 9 | 0.81 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 20 | 0.81 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 20 | 0.81 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 20 | 0.81 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 20 | 0.81 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 20 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 20 | 0.81 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 5 | 0.81 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 5 | 0.81 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 5 | 0.81 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 4 | 0.81 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 13 | 0.81 |
| (1,1412) | 1:174:A:GLU:HG2 | 1:177:A:GLU:HB3 | 7 | 0.81 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 16 | 0.81 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 16 | 0.81 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 16 | 0.81 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 20 | 0.81 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 20 | 0.81 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 20 | 0.81 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 8 | 0.81 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 8 | 0.81 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 2 | 0.81 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 20 | 0.81 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 5 | 0.81 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 17 | 0.81 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 7 | 0.81 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 3 | 0.81 |
| (1,609) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 6 | 0.81 |
| (1,609) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 6 | 0.81 |
| (1,609) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 6 | 0.81 |
| (1,468) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 3 | 0.81 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 10 | 0.81 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 11 | 0.81 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 11 | 0.81 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 6 | 0.81 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 6 | 0.81 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 6 | 0.81 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 6 | 0.81 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 3 | 0.81 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 3 | 0.81 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 3 | 0.81 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 7 | 0.81 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 7 | 0.81 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 7 | 0.81 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 14 | 0.81 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 14 | 0.81 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 14 | 0.81 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 11 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 11 | 0.81 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 11 | 0.81 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 10 | 0.81 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 10 | 0.81 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 10 | 0.81 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 5 | 0.8 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 5 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 14 | 0.8 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 14 | 0.8 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 4 | 0.8 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 4 | 0.8 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 4 | 0.8 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 4 | 0.8 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 4 | 0.8 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 4 | 0.8 |
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 19 | 0.8 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 19 | 0.8 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 8 | 0.8 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 8 | 0.8 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 8 | 0.8 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 9 | 0.8 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 12 | 0.8 |
| (1,3405) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HB3 | 8 | 0.8 |
| (1,3405) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HB3 | 8 | 0.8 |
| (1,3405) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HB3 | 8 | 0.8 |
| (1,3249) | 1:143:A:VAL:HB | 1:182:A:HIS:HE1 | 13 | 0.8 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 1 | 0.8 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 1 | 0.8 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 13 | 0.8 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 13 | 0.8 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 1 | 0.8 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 1 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 1 | 0.8 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 15 | 0.8 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 9 | 0.8 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 1 | 0.8 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 1 | 0.8 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 1 | 0.8 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 19 | 0.8 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 5 | 0.8 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 12 | 0.8 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 4 | 0.8 |
| (1,2123) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 19 | 0.8 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 18 | 0.8 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 18 | 0.8 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 18 | 0.8 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 7 | 0.8 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 7 | 0.8 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 7 | 0.8 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 2 | 0.8 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 17 | 0.8 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 1 | 0.8 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 1 | 0.8 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 1 | 0.8 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 1 | 0.8 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 1 | 0.8 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 1 | 0.8 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 17 | 0.8 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD11 | 3 | 0.8 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD12 | 3 | 0.8 |
| (1,1431) | 1:177:A:GLU:HA | 1:209:A:LEU:HD13 | 3 | 0.8 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 2 | 0.8 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 19 | 0.8 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 19 | 0.8 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 4 | 0.8 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 6 | 0.8 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 19 | 0.8 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 5 | 0.8 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 5 | 0.8 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 5 | 0.8 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 5 | 0.8 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 5 | 0.8 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 5 | 0.8 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 20 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 20 | 0.8 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 20 | 0.8 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 20 | 0.8 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 20 | 0.8 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 20 | 0.8 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 10 | 0.8 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 10 | 0.8 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 10 | 0.8 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 3 | 0.8 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 3 | 0.8 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 3 | 0.8 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 9 | 0.8 |
| (1,609) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 1 | 0.8 |
| (1,609) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 1 | 0.8 |
| (1,609) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 1 | 0.8 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 19 | 0.8 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 19 | 0.8 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 19 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 11 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 11 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 11 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 11 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 11 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 11 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 18 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 18 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 18 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 18 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 18 | 0.8 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 18 | 0.8 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 3 | 0.8 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 6 | 0.8 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 9 | 0.8 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 17 | 0.8 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 16 | 0.8 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 16 | 0.8 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 16 | 0.8 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 17 | 0.8 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 17 | 0.8 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 17 | 0.8 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 12 | 0.8 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 4 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 15 | 0.8 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 16 | 0.79 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 16 | 0.79 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 16 | 0.79 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 16 | 0.79 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 16 | 0.79 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 16 | 0.79 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 3 | 0.79 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 3 | 0.79 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 16 | 0.79 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 16 | 0.79 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 5 | 0.79 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 5 | 0.79 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 5 | 0.79 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 5 | 0.79 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 5 | 0.79 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 5 | 0.79 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 15 | 0.79 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 17 | 0.79 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 3 | 0.79 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 3 | 0.79 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 11 | 0.79 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 20 | 0.79 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 2 | 0.79 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 2 | 0.79 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 5 | 0.79 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 1 | 0.79 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 12 | 0.79 |
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 8 | 0.79 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 8 | 0.79 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 16 | 0.79 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 16 | 0.79 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 11 | 0.79 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 20 | 0.79 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 10 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 17 | 0.79 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 17 | 0.79 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 20 | 0.79 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 20 | 0.79 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 7 | 0.79 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 7 | 0.79 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 7 | 0.79 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 18 | 0.79 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 18 | 0.79 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 18 | 0.79 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 5 | 0.79 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 13 | 0.79 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 4 | 0.79 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 4 | 0.79 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 4 | 0.79 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 3 | 0.79 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 3 | 0.79 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 3 | 0.79 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD11 | 12 | 0.79 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD12 | 12 | 0.79 |
| (1,2010) | 1:215:A:GLU:H | 1:216:A:LEU:HD13 | 12 | 0.79 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 1 | 0.79 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 20 | 0.79 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 20 | 0.79 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 20 | 0.79 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 7 | 0.79 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 3 | 0.79 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 8 | 0.79 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 8 | 0.79 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 8 | 0.79 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 8 | 0.79 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 8 | 0.79 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 8 | 0.79 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 2 | 0.79 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 17 | 0.79 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 17 | 0.79 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 17 | 0.79 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 12 | 0.79 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 12 | 0.79 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 12 | 0.79 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 8 | 0.79 |
| (1,1413) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB3 | 1 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 12 | 0.79 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 12 | 0.79 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 12 | 0.79 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 14 | 0.79 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 14 | 0.79 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 16 | 0.79 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 16 | 0.79 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 3 | 0.79 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 5 | 0.79 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 5 | 0.79 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 5 | 0.79 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 5 | 0.79 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 5 | 0.79 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 5 | 0.79 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 1 | 0.79 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 1 | 0.79 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 11 | 0.79 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 18 | 0.79 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 18 | 0.79 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 10 | 0.79 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 15 | 0.79 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 13 | 0.79 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 15 | 0.79 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 15 | 0.79 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 15 | 0.79 |
| (1,762) | 1:83:A:GLN:HB3 | 1:111:A:HIS:HB2 | 15 | 0.79 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 12 | 0.79 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 12 | 0.79 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 16 | 0.79 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 20 | 0.79 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 20 | 0.79 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 20 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 20 | 0.79 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 20 | 0.79 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 20 | 0.79 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 18 | 0.79 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 18 | 0.79 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 18 | 0.79 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 15 | 0.79 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 15 | 0.79 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 15 | 0.79 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 2 | 0.79 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 2 | 0.79 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 2 | 0.79 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 11 | 0.79 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 19 | 0.78 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 19 | 0.78 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 19 | 0.78 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 19 | 0.78 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD21 | 2 | 0.78 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD22 | 2 | 0.78 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 5 | 0.78 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 5 | 0.78 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 20 | 0.78 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 20 | 0.78 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 8 | 0.78 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 14 | 0.78 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 14 | 0.78 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 14 | 0.78 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 14 | 0.78 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 14 | 0.78 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 8 | 0.78 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 8 | 0.78 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 8 | 0.78 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 8 | 0.78 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 8 | 0.78 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 8 | 0.78 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 18 | 0.78 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 6 | 0.78 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 6 | 0.78 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 8 | 0.78 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 10 | 0.78 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 2 | 0.78 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 2 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 2 | 0.78 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 1 | 0.78 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 1 | 0.78 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 1 | 0.78 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 8 | 0.78 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 5 | 0.78 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 5 | 0.78 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 19 | 0.78 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 19 | 0.78 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 19 | 0.78 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 19 | 0.78 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 6 | 0.78 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 6 | 0.78 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 3 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 4 | 0.78 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 4 | 0.78 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 6 | 0.78 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 6 | 0.78 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 6 | 0.78 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 8 | 0.78 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 8 | 0.78 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 8 | 0.78 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 3 | 0.78 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 17 | 0.78 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 15 | 0.78 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 15 | 0.78 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 15 | 0.78 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 15 | 0.78 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 15 | 0.78 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 15 | 0.78 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 1 | 0.78 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 1 | 0.78 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 1 | 0.78 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 15 | 0.78 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 15 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 7 | 0.78 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 7 | 0.78 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 2 | 0.78 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 2 | 0.78 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 2 | 0.78 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 20 | 0.78 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 20 | 0.78 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 20 | 0.78 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 20 | 0.78 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 20 | 0.78 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 20 | 0.78 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 16 | 0.78 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 16 | 0.78 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 16 | 0.78 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 16 | 0.78 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 16 | 0.78 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 16 | 0.78 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 17 | 0.78 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 17 | 0.78 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 17 | 0.78 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 8 | 0.78 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 17 | 0.78 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB1 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB2 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB3 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB1 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB2 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB3 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB1 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB2 | 12 | 0.78 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB3 | 12 | 0.78 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 12 | 0.78 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 15 | 0.78 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 1 | 0.78 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 15 | 0.78 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 14 | 0.78 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 2 | 0.78 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 11 | 0.78 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 7 | 0.78 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 7 | 0.78 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 7 | 0.78 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 7 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 7 | 0.78 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 7 | 0.78 |
| (1,580) | 1:91:A:GLN:HA | 1:92:A:LYS:HG2 | 17 | 0.78 |
| (1,580) | 1:91:A:GLN:HA | 1:92:A:LYS:HG3 | 17 | 0.78 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 3 | 0.78 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 3 | 0.78 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 3 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 10 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 10 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 10 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 10 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 10 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 10 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 15 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 15 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 15 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 15 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 15 | 0.78 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 15 | 0.78 |
| (1,446) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA3 | 16 | 0.78 |
| (1,446) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA3 | 16 | 0.78 |
| (1,446) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA3 | 16 | 0.78 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 12 | 0.78 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 12 | 0.78 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 12 | 0.78 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 17 | 0.78 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 17 | 0.78 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 17 | 0.78 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 17 | 0.78 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 1 | 0.78 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 7 | 0.77 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 7 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 20 | 0.77 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 20 | 0.77 |
| (1,3616) | 1:80:A:SER:HB2 | 1:114:A:ASP:HB2 | 5 | 0.77 |
| (1,3616) | 1:80:A:SER:HB2 | 1:114:A:ASP:HB3 | 5 | 0.77 |
| (1,3616) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB2 | 5 | 0.77 |
| (1,3616) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB3 | 5 | 0.77 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 8 | 0.77 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 8 | 0.77 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 9 | 0.77 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 9 | 0.77 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 9 | 0.77 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 9 | 0.77 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG21 | 5 | 0.77 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG22 | 5 | 0.77 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG23 | 5 | 0.77 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG21 | 5 | 0.77 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG22 | 5 | 0.77 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG23 | 5 | 0.77 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 5 | 0.77 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 5 | 0.77 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 5 | 0.77 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 5 | 0.77 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 5 | 0.77 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 5 | 0.77 |
| (1,3474) | 2:17:B:LYS:HD2 | 2:18:B:CYS:H | 15 | 0.77 |
| (1,3474) | 2:17:B:LYS:HD3 | 2:18:B:CYS:H | 15 | 0.77 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 14 | 0.77 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 14 | 0.77 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 17 | 0.77 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 17 | 0.77 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 17 | 0.77 |
| (1,3206) | 1:88:A:GLN:HG2 | 1:90:A:HIS:HE1 | 5 | 0.77 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 18 | 0.77 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 18 | 0.77 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 14 | 0.77 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 7 | 0.77 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 12 | 0.77 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 14 | 0.77 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 20 | 0.77 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 7 | 0.77 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 19 | 0.77 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 7 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 7 | 0.77 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 7 | 0.77 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD11 | 3 | 0.77 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD12 | 3 | 0.77 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD13 | 3 | 0.77 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 9 | 0.77 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 9 | 0.77 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 9 | 0.77 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 19 | 0.77 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 19 | 0.77 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 19 | 0.77 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 16 | 0.77 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 18 | 0.77 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 18 | 0.77 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 18 | 0.77 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 18 | 0.77 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 18 | 0.77 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 18 | 0.77 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 17 | 0.77 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 17 | 0.77 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 17 | 0.77 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 13 | 0.77 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 13 | 0.77 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 3 | 0.77 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 3 | 0.77 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 3 | 0.77 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 3 | 0.77 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 3 | 0.77 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 3 | 0.77 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 3 | 0.77 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 20 | 0.77 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 4 | 0.77 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 4 | 0.77 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 4 | 0.77 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 12 | 0.77 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 12 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 12 | 0.77 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 12 | 0.77 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 12 | 0.77 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 12 | 0.77 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 1 | 0.77 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 1 | 0.77 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 1 | 0.77 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 1 | 0.77 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 2 | 0.77 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 5 | 0.77 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 3 | 0.77 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 3 | 0.77 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 3 | 0.77 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 17 | 0.77 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 17 | 0.77 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 17 | 0.77 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD21 | 12 | 0.77 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD22 | 12 | 0.77 |
| (1,1227) | 1:184:A:ILE:HB | 1:216:A:LEU:HD23 | 12 | 0.77 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 17 | 0.77 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 17 | 0.77 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 17 | 0.77 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG21 | 5 | 0.77 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG22 | 5 | 0.77 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG23 | 5 | 0.77 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 1 | 0.77 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 1 | 0.77 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 1 | 0.77 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 9 | 0.77 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 11 | 0.77 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 5 | 0.77 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 5 | 0.77 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 5 | 0.77 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 5 | 0.77 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 5 | 0.77 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 5 | 0.77 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 9 | 0.77 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 9 | 0.77 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 9 | 0.77 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 9 | 0.77 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 9 | 0.77 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 9 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 20 | 0.77 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 7 | 0.77 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 7 | 0.77 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 5 | 0.77 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 20 | 0.77 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 13 | 0.77 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 13 | 0.77 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 13 | 0.77 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 11 | 0.77 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 11 | 0.77 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 11 | 0.77 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 17 | 0.77 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 16 | 0.77 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 16 | 0.77 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 16 | 0.77 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 16 | 0.77 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 16 | 0.77 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 16 | 0.77 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 3 | 0.77 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 12 | 0.77 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 12 | 0.77 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 12 | 0.77 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 4 | 0.77 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 4 | 0.77 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 11 | 0.77 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 11 | 0.77 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 15 | 0.76 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 15 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 2 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 8 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 8 | 0.76 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 8 | 0.76 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE21 | 4 | 0.76 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE22 | 4 | 0.76 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 7 | 0.76 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 7 | 0.76 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 7 | 0.76 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 7 | 0.76 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 6 | 0.76 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 11 | 0.76 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 11 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 16 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 16 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 16 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 16 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 16 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 16 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 19 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 19 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 19 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 19 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 19 | 0.76 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 19 | 0.76 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 8 | 0.76 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 18 | 0.76 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 16 | 0.76 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 2 | 0.76 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 10 | 0.76 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 20 | 0.76 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 4 | 0.76 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 11 | 0.76 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 13 | 0.76 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 7 | 0.76 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 15 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 15 | 0.76 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 15 | 0.76 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 10 | 0.76 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 10 | 0.76 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 10 | 0.76 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 15 | 0.76 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 15 | 0.76 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 15 | 0.76 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 15 | 0.76 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 15 | 0.76 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 15 | 0.76 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 16 | 0.76 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 16 | 0.76 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 16 | 0.76 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB1 | 11 | 0.76 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB2 | 11 | 0.76 |
| (1,1410) | 1:174:A:GLU:HG2 | 1:178:A:ALA:HB3 | 11 | 0.76 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 3 | 0.76 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 10 | 0.76 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 10 | 0.76 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 12 | 0.76 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 12 | 0.76 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 12 | 0.76 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 4 | 0.76 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 18 | 0.76 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 18 | 0.76 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 18 | 0.76 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 15 | 0.76 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 15 | 0.76 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 15 | 0.76 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 15 | 0.76 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 15 | 0.76 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 15 | 0.76 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 7 | 0.76 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 9 | 0.76 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 17 | 0.76 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 6 | 0.76 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 1 | 0.76 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 1 | 0.76 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 1 | 0.76 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 1 | 0.76 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 1 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 1 | 0.76 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 16 | 0.76 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 16 | 0.76 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 16 | 0.76 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 11 | 0.76 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 11 | 0.76 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 13 | 0.76 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 19 | 0.76 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 19 | 0.76 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 2 | 0.76 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 20 | 0.76 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 6 | 0.76 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 6 | 0.76 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 6 | 0.76 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 14 | 0.76 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 4 | 0.76 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 17 | 0.76 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 17 | 0.76 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 17 | 0.76 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 17 | 0.76 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 6 | 0.75 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 6 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 13 | 0.75 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 13 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 16 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 16 | 0.75 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 16 | 0.75 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 20 | 0.75 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 20 | 0.75 |
| (1,3530) | 1:63:A:TYR:HE1 | 2:21:B:MET:HB2 | 2 | 0.75 |
| (1,3530) | 1:63:A:TYR:HE2 | 2:21:B:MET:HB2 | 2 | 0.75 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 8 | 0.75 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 15 | 0.75 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 14 | 0.75 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 1 | 0.75 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 1 | 0.75 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 1 | 0.75 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 11 | 0.75 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 3 | 0.75 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 16 | 0.75 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 2 | 0.75 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 7 | 0.75 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 20 | 0.75 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 4 | 0.75 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 4 | 0.75 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 4 | 0.75 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 6 | 0.75 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 6 | 0.75 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 6 | 0.75 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 9 | 0.75 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD11 | 3 | 0.75 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD12 | 3 | 0.75 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD13 | 3 | 0.75 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD21 | 3 | 0.75 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD22 | 3 | 0.75 |
| (1,2841) | 1:178:A:ALA:H | 1:179:A:LEU:HD23 | 3 | 0.75 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 6 | 0.75 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 8 | 0.75 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 17 | 0.75 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 5 | 0.75 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 5 | 0.75 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 5 | 0.75 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 12 | 0.75 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 12 | 0.75 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 12 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 15 | 0.75 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 15 | 0.75 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 15 | 0.75 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 8 | 0.75 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 8 | 0.75 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 8 | 0.75 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 13 | 0.75 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 8 | 0.75 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 16 | 0.75 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 16 | 0.75 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 16 | 0.75 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 14 | 0.75 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 10 | 0.75 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 8 | 0.75 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 8 | 0.75 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 8 | 0.75 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 17 | 0.75 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 17 | 0.75 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 17 | 0.75 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 4 | 0.75 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 4 | 0.75 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 4 | 0.75 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 10 | 0.75 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 10 | 0.75 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 10 | 0.75 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 11 | 0.75 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 11 | 0.75 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 11 | 0.75 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 18 | 0.75 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 18 | 0.75 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 18 | 0.75 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 18 | 0.75 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 18 | 0.75 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 18 | 0.75 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 16 | 0.75 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 1 | 0.75 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 12 | 0.75 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 20 | 0.75 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 20 | 0.75 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 20 | 0.75 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 6 | 0.75 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 6 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 6 | 0.75 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 6 | 0.75 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 6 | 0.75 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 6 | 0.75 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 8 | 0.75 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 8 | 0.75 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 8 | 0.75 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 14 | 0.75 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 14 | 0.75 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 14 | 0.75 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 13 | 0.75 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 13 | 0.75 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 13 | 0.75 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 12 | 0.75 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 1 | 0.75 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 1 | 0.75 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 1 | 0.75 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 6 | 0.75 |
| (1,167) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HD22 | 13 | 0.75 |
| (1,167) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HD22 | 13 | 0.75 |
| (1,167) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HD22 | 13 | 0.75 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 10 | 0.75 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 17 | 0.75 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 18 | 0.75 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 18 | 0.75 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 18 | 0.75 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 11 | 0.75 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 11 | 0.75 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 11 | 0.75 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 11 | 0.75 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 11 | 0.75 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 11 | 0.75 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 6 | 0.75 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 8 | 0.75 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 11 | 0.75 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 14 | 0.74 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 14 | 0.74 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 14 | 0.74 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 14 | 0.74 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 14 | 0.74 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 14 | 0.74 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 16 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 16 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 3 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 3 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 3 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 3 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 3 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 3 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 12 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 12 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 12 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 12 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 12 | 0.74 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 12 | 0.74 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 9 | 0.74 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 19 | 0.74 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 19 | 0.74 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 14 | 0.74 |
| (1,3218) | 1:119:A:LEU:HD11 | 1:133:A:TRP:HZ2 | 19 | 0.74 |
| (1,3218) | 1:119:A:LEU:HD12 | 1:133:A:TRP:HZ2 | 19 | 0.74 |
| (1,3218) | 1:119:A:LEU:HD13 | 1:133:A:TRP:HZ2 | 19 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 3 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 3 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 3 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 3 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 3 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 3 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 13 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 13 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 13 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 13 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 13 | 0.74 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 13 | 0.74 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 9 | 0.74 |
| (1,3091) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 4 | 0.74 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 15 | 0.74 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 17 | 0.74 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 18 | 0.74 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 13 | 0.74 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 7 | 0.74 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 7 | 0.74 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 7 | 0.74 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 3 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 13 | 0.74 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 19 | 0.74 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 19 | 0.74 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 19 | 0.74 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 6 | 0.74 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 19 | 0.74 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 17 | 0.74 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 13 | 0.74 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 13 | 0.74 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 1 | 0.74 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 1 | 0.74 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 1 | 0.74 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 9 | 0.74 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 4 | 0.74 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 4 | 0.74 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 4 | 0.74 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 4 | 0.74 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG12 | 8 | 0.74 |
| (1,1810) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG13 | 8 | 0.74 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 18 | 0.74 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 18 | 0.74 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 18 | 0.74 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 19 | 0.74 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 19 | 0.74 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 19 | 0.74 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 19 | 0.74 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 19 | 0.74 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 19 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 2 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 2 | 0.74 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 2 | 0.74 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 1 | 0.74 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 1 | 0.74 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 1 | 0.74 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 5 | 0.74 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 5 | 0.74 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 20 | 0.74 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 20 | 0.74 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 20 | 0.74 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 5 | 0.74 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 20 | 0.74 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 10 | 0.74 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 3 | 0.74 |
| (1,896) | 1:123:A:LYS:HE3 | 1:136:A:TYR:HB3 | 4 | 0.74 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 14 | 0.74 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 14 | 0.74 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 12 | 0.74 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 19 | 0.74 |
| (1,643) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 20 | 0.74 |
| (1,580) | 1:91:A:GLN:HA | 1:92:A:LYS:HG2 | 3 | 0.74 |
| (1,580) | 1:91:A:GLN:HA | 1:92:A:LYS:HG3 | 3 | 0.74 |
| (1,468) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 8 | 0.74 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 7 | 0.74 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 7 | 0.74 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 7 | 0.74 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 9 | 0.74 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 9 | 0.74 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 9 | 0.74 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 12 | 0.74 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 3 | 0.74 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 3 | 0.74 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 3 | 0.74 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 3 | 0.74 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 3 | 0.74 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 3 | 0.74 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 20 | 0.74 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 20 | 0.74 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 20 | 0.74 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 14 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 12 | 0.74 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 4 | 0.74 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 4 | 0.74 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 4 | 0.74 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 2 | 0.73 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 2 | 0.73 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 2 | 0.73 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 2 | 0.73 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 2 | 0.73 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 2 | 0.73 |
| (1,3683) | 1:94:A:ALA:H | 1:97:A:GLN:HB2 | 11 | 0.73 |
| (1,3683) | 1:94:A:ALA:H | 1:97:A:GLN:HB3 | 11 | 0.73 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 1 | 0.73 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 1 | 0.73 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 13 | 0.73 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 13 | 0.73 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 6 | 0.73 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 12 | 0.73 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 12 | 0.73 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 8 | 0.73 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 8 | 0.73 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 8 | 0.73 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 8 | 0.73 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 8 | 0.73 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 8 | 0.73 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 19 | 0.73 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 19 | 0.73 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 19 | 0.73 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 19 | 0.73 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 5 | 0.73 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 3 | 0.73 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 6 | 0.73 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 15 | 0.73 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 2 | 0.73 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 12 | 0.73 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 4 | 0.73 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 9 | 0.73 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 9 | 0.73 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 2 | 0.73 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 2 | 0.73 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 2 | 0.73 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 6 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 6 | 0.73 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 6 | 0.73 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 8 | 0.73 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 8 | 0.73 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 8 | 0.73 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 9 | 0.73 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 9 | 0.73 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 2 | 0.73 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 2 | 0.73 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 2 | 0.73 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 16 | 0.73 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 16 | 0.73 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 16 | 0.73 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 9 | 0.73 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 5 | 0.73 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 5 | 0.73 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 5 | 0.73 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 20 | 0.73 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 20 | 0.73 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 20 | 0.73 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 10 | 0.73 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 10 | 0.73 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 17 | 0.73 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 17 | 0.73 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 17 | 0.73 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 7 | 0.73 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 7 | 0.73 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 7 | 0.73 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 7 | 0.73 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 7 | 0.73 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 7 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 5 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 5 | 0.73 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 5 | 0.73 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 7 | 0.73 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 8 | 0.73 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 8 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 6 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 6 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 6 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 8 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 8 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 8 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 15 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 15 | 0.73 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 15 | 0.73 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 17 | 0.73 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 5 | 0.73 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 5 | 0.73 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 5 | 0.73 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 19 | 0.73 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 19 | 0.73 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 19 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 19 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 19 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 19 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 19 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 19 | 0.73 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 19 | 0.73 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 7 | 0.73 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 13 | 0.73 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 14 | 0.73 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 20 | 0.73 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 1 | 0.73 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 6 | 0.73 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 6 | 0.73 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 6 | 0.73 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 13 | 0.73 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 18 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 10 | 0.73 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 10 | 0.73 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 10 | 0.73 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 10 | 0.73 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 10 | 0.73 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 10 | 0.73 |
| (1,595) | 1:141:A:GLU:HG2 | 1:148:A:SER:HA | 7 | 0.73 |
| (1,595) | 1:141:A:GLU:HG3 | 1:148:A:SER:HA | 7 | 0.73 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG11 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG12 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG13 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG21 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG22 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG23 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG11 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG12 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG13 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG21 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG22 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG23 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG11 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG12 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG13 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG21 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG22 | 14 | 0.73 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG23 | 14 | 0.73 |
| (1,453) | 1:158:A:ASP:HB3 | 1:160:A:GLY:HA3 | 18 | 0.73 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 19 | 0.73 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 19 | 0.73 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 19 | 0.73 |
| (1,232) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 20 | 0.73 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 2 | 0.73 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 1 | 0.73 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 1 | 0.73 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 1 | 0.73 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 5 | 0.73 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 12 | 0.73 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 18 | 0.73 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 11 | 0.72 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 11 | 0.72 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 6 | 0.72 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 6 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 6 | 0.72 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 6 | 0.72 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 6 | 0.72 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 6 | 0.72 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 9 | 0.72 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 9 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 1 | 0.72 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 1 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 9 | 0.72 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 9 | 0.72 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 11 | 0.72 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 11 | 0.72 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 11 | 0.72 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 11 | 0.72 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 11 | 0.72 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 11 | 0.72 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 12 | 0.72 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 12 | 0.72 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 7 | 0.72 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 7 | 0.72 |
| (1,3496) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HA | 13 | 0.72 |
| (1,3496) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HA | 13 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3496) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HA | 13 | 0.72 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 6 | 0.72 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 6 | 0.72 |
| (1,3265) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HG2 | 2 | 0.72 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 10 | 0.72 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 10 | 0.72 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 10 | 0.72 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 10 | 0.72 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 10 | 0.72 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 10 | 0.72 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 16 | 0.72 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 7 | 0.72 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 11 | 0.72 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 11 | 0.72 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 11 | 0.72 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 11 | 0.72 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 18 | 0.72 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 18 | 0.72 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 18 | 0.72 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 13 | 0.72 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 18 | 0.72 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 4 | 0.72 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 5 | 0.72 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 5 | 0.72 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 5 | 0.72 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 19 | 0.72 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 14 | 0.72 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 9 | 0.72 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 9 | 0.72 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 9 | 0.72 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 19 | 0.72 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 17 | 0.72 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 17 | 0.72 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 17 | 0.72 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 10 | 0.72 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 19 | 0.72 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 13 | 0.72 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 13 | 0.72 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 13 | 0.72 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 13 | 0.72 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 13 | 0.72 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 13 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 20 | 0.72 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 20 | 0.72 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 20 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 11 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 11 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 11 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 11 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 11 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 11 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 16 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 16 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 16 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 16 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 16 | 0.72 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 16 | 0.72 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 12 | 0.72 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 12 | 0.72 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 12 | 0.72 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 10 | 0.72 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 10 | 0.72 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 10 | 0.72 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 2 | 0.72 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 2 | 0.72 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 2 | 0.72 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 3 | 0.72 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 3 | 0.72 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 3 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 19 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 19 | 0.72 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 19 | 0.72 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 1 | 0.72 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 1 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 14 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 14 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 14 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 20 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 20 | 0.72 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 20 | 0.72 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 12 | 0.72 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 12 | 0.72 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 12 | 0.72 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 17 | 0.72 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 17 | 0.72 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 17 | 0.72 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 7 | 0.72 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 7 | 0.72 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 14 | 0.72 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 14 | 0.72 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 14 | 0.72 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 16 | 0.72 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 16 | 0.72 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 16 | 0.72 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 7 | 0.72 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 18 | 0.72 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 5 | 0.72 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 19 | 0.72 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 19 | 0.72 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 19 | 0.72 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 5 | 0.72 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 5 | 0.72 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 5 | 0.72 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 17 | 0.72 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 9 | 0.72 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 9 | 0.72 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 10 | 0.72 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 10 | 0.72 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 3 | 0.72 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 3 | 0.72 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 3 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 10 | 0.72 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 10 | 0.72 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 10 | 0.72 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 20 | 0.72 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 20 | 0.72 |
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 20 | 0.72 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 20 | 0.72 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 20 | 0.72 |
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 20 | 0.72 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD11 | 3 | 0.72 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD12 | 3 | 0.72 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD13 | 3 | 0.72 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 1 | 0.72 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 1 | 0.72 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 1 | 0.72 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 12 | 0.72 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 1 | 0.71 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 1 | 0.71 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 1 | 0.71 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 1 | 0.71 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 1 | 0.71 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 1 | 0.71 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 14 | 0.71 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 14 | 0.71 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 14 | 0.71 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 14 | 0.71 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 14 | 0.71 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 14 | 0.71 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 1 | 0.71 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 1 | 0.71 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 1 | 0.71 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 1 | 0.71 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 1 | 0.71 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 1 | 0.71 |
| (1,3564) | 1:62:A:ASP:H | 1:66:A:ASP:HB2 | 12 | 0.71 |
| (1,3564) | 1:62:A:ASP:H | 1:66:A:ASP:HB3 | 12 | 0.71 |
| (1,3486) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HA | 13 | 0.71 |
| (1,3486) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HA | 13 | 0.71 |
| (1,3486) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HA | 13 | 0.71 |
| (1,3486) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HA | 16 | 0.71 |
| (1,3486) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HA | 16 | 0.71 |
| (1,3486) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HA | 16 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 10 | 0.71 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 10 | 0.71 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 10 | 0.71 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 17 | 0.71 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 17 | 0.71 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 17 | 0.71 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 17 | 0.71 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 17 | 0.71 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 17 | 0.71 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 18 | 0.71 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 10 | 0.71 |
| (1,3248) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HE1 | 19 | 0.71 |
| (1,3248) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HE1 | 19 | 0.71 |
| (1,3248) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HE1 | 19 | 0.71 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 16 | 0.71 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 16 | 0.71 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 19 | 0.71 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 10 | 0.71 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 6 | 0.71 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 18 | 0.71 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 18 | 0.71 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 4 | 0.71 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 11 | 0.71 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 15 | 0.71 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 16 | 0.71 |
| (1,2811) | 1:174:A:GLU:HB3 | 1:175:A:ASN:H | 17 | 0.71 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 1 | 0.71 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 2 | 0.71 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 11 | 0.71 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 13 | 0.71 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 18 | 0.71 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 5 | 0.71 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 5 | 0.71 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 5 | 0.71 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 5 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 6 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 6 | 0.71 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 6 | 0.71 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 2 | 0.71 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD11 | 12 | 0.71 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD12 | 12 | 0.71 |
| (1,2006) | 1:215:A:GLU:HG2 | 1:216:A:LEU:HD13 | 12 | 0.71 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 7 | 0.71 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 7 | 0.71 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 7 | 0.71 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 17 | 0.71 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 17 | 0.71 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 17 | 0.71 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 17 | 0.71 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 17 | 0.71 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 17 | 0.71 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 14 | 0.71 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 14 | 0.71 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 14 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 13 | 0.71 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 13 | 0.71 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 10 | 0.71 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 10 | 0.71 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 12 | 0.71 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 12 | 0.71 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 14 | 0.71 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 14 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 4 | 0.71 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 4 | 0.71 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 4 | 0.71 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 1 | 0.71 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 11 | 0.71 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 17 | 0.71 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 17 | 0.71 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 17 | 0.71 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 16 | 0.71 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 17 | 0.71 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 19 | 0.71 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 19 | 0.71 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 19 | 0.71 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 18 | 0.71 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 18 | 0.71 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 18 | 0.71 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 18 | 0.71 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 18 | 0.71 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 18 | 0.71 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 2 | 0.71 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 2 | 0.71 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 6 | 0.71 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 11 | 0.71 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 11 | 0.71 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 11 | 0.71 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 11 | 0.71 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 11 | 0.71 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 11 | 0.71 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 6 | 0.71 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 19 | 0.71 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 19 | 0.71 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 14 | 0.71 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 13 | 0.71 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 13 | 0.71 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 13 | 0.71 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 9 | 0.71 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 9 | 0.71 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 9 | 0.71 |
| (1,330) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HA | 3 | 0.71 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 3 | 0.71 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 2 | 0.71 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 2 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 2 | 0.71 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 2 | 0.71 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 2 | 0.71 |
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 2 | 0.71 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 9 | 0.71 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 11 | 0.71 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 1 | 0.71 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD21 | 5 | 0.7 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD22 | 5 | 0.7 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 12 | 0.7 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 12 | 0.7 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 12 | 0.7 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 12 | 0.7 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 12 | 0.7 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 12 | 0.7 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 3 | 0.7 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 3 | 0.7 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 3 | 0.7 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 3 | 0.7 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 3 | 0.7 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 3 | 0.7 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD21 | 6 | 0.7 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD22 | 6 | 0.7 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD21 | 6 | 0.7 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD22 | 6 | 0.7 |
| (1,3703) | 1:102:A:ARG:H | 1:129:A:ASN:HD21 | 10 | 0.7 |
| (1,3703) | 1:102:A:ARG:H | 1:129:A:ASN:HD22 | 10 | 0.7 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 2 | 0.7 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 2 | 0.7 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 10 | 0.7 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 10 | 0.7 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 7 | 0.7 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 7 | 0.7 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 7 | 0.7 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 11 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 11 | 0.7 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 11 | 0.7 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 1 | 0.7 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 1 | 0.7 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 1 | 0.7 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 12 | 0.7 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 13 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 7 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 7 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 7 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 7 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 7 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 7 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 11 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 11 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 11 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 11 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 11 | 0.7 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 11 | 0.7 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 13 | 0.7 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 8 | 0.7 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 9 | 0.7 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 9 | 0.7 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 9 | 0.7 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD11 | 2 | 0.7 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD12 | 2 | 0.7 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD13 | 2 | 0.7 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 15 | 0.7 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 15 | 0.7 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 15 | 0.7 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 15 | 0.7 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 4 | 0.7 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 1 | 0.7 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 10 | 0.7 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 10 | 0.7 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 10 | 0.7 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 14 | 0.7 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 14 | 0.7 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 14 | 0.7 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 11 | 0.7 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 11 | 0.7 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 11 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 14 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 14 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 14 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 14 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 14 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 14 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 17 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 17 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 17 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 17 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 17 | 0.7 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 17 | 0.7 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 15 | 0.7 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 15 | 0.7 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 13 | 0.7 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 13 | 0.7 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 13 | 0.7 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 19 | 0.7 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 19 | 0.7 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 19 | 0.7 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 9 | 0.7 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 20 | 0.7 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD11 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD12 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD13 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD21 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD22 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD23 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD11 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD12 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD13 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD21 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD22 | 19 | 0.7 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD23 | 19 | 0.7 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 17 | 0.7 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 17 | 0.7 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 17 | 0.7 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 17 | 0.7 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 17 | 0.7 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 17 | 0.7 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 10 | 0.7 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 13 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 13 | 0.7 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 13 | 0.7 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 13 | 0.7 |
| (1,468) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 16 | 0.7 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 16 | 0.7 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 16 | 0.7 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 16 | 0.7 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 11 | 0.7 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 11 | 0.7 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 11 | 0.7 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 15 | 0.7 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 15 | 0.7 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 15 | 0.7 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 20 | 0.7 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 20 | 0.7 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 20 | 0.7 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 4 | 0.7 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 14 | 0.7 |
| (1,183) | 1:58:A:HIS:HB3 | 2:12:B:ASN:HD22 | 1 | 0.7 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 8 | 0.7 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 8 | 0.7 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 8 | 0.7 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 18 | 0.7 |
| (1,15) | 1:47:A:THR:HB | 1:48:A:ASN:HB2 | 17 | 0.7 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 15 | 0.7 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 6 | 0.69 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 6 | 0.69 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 7 | 0.69 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 7 | 0.69 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 19 | 0.69 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 19 | 0.69 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 19 | 0.69 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 19 | 0.69 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 19 | 0.69 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 19 | 0.69 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB2 | 15 | 0.69 |
| (1,3711) | 1:103:A:THR:HG21 | 1:128:A:LEU:HB3 | 15 | 0.69 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB2 | 15 | 0.69 |
| (1,3711) | 1:103:A:THR:HG22 | 1:128:A:LEU:HB3 | 15 | 0.69 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB2 | 15 | 0.69 |
| (1,3711) | 1:103:A:THR:HG23 | 1:128:A:LEU:HB3 | 15 | 0.69 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 10 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 10 | 0.69 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 10 | 0.69 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 10 | 0.69 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 10 | 0.69 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 10 | 0.69 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 12 | 0.69 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 12 | 0.69 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 12 | 0.69 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 12 | 0.69 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE21 | 15 | 0.69 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE22 | 15 | 0.69 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 11 | 0.69 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 11 | 0.69 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 2 | 0.69 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 2 | 0.69 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 2 | 0.69 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 2 | 0.69 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 2 | 0.69 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 2 | 0.69 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 8 | 0.69 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 8 | 0.69 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 8 | 0.69 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 8 | 0.69 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 8 | 0.69 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 8 | 0.69 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 20 | 0.69 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 2 | 0.69 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 2 | 0.69 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 2 | 0.69 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 1 | 0.69 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 1 | 0.69 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 1 | 0.69 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 16 | 0.69 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 16 | 0.69 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 16 | 0.69 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 8 | 0.69 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 8 | 0.69 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 17 | 0.69 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 17 | 0.69 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 17 | 0.69 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 18 | 0.69 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 11 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3192) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HB | 9 | 0.69 |
| (1,3192) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HB | 9 | 0.69 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 7 | 0.69 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 7 | 0.69 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 8 | 0.69 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 8 | 0.69 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 20 | 0.69 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 20 | 0.69 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 14 | 0.69 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 14 | 0.69 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 14 | 0.69 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 14 | 0.69 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 14 | 0.69 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 14 | 0.69 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 15 | 0.69 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 15 | 0.69 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 15 | 0.69 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 8 | 0.69 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 3 | 0.69 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 7 | 0.69 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 8 | 0.69 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 15 | 0.69 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 10 | 0.69 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 10 | 0.69 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 10 | 0.69 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 13 | 0.69 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 13 | 0.69 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 13 | 0.69 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 18 | 0.69 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD11 | 8 | 0.69 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD12 | 8 | 0.69 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD13 | 8 | 0.69 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 15 | 0.69 |
| (1,2229) | 1:66:A:ASP:H | 1:67:A:ALA:H | 12 | 0.69 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 14 | 0.69 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 1 | 0.69 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 1 | 0.69 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 1 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 13 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 13 | 0.69 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 13 | 0.69 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD11 | 19 | 0.69 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD12 | 19 | 0.69 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD13 | 19 | 0.69 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD21 | 3 | 0.69 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD22 | 3 | 0.69 |
| (1,1925) | 1:206:A:ALA:HA | 1:209:A:LEU:HD23 | 3 | 0.69 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 12 | 0.69 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 15 | 0.69 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 3 | 0.69 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 3 | 0.69 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 3 | 0.69 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 18 | 0.69 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 18 | 0.69 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 18 | 0.69 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 9 | 0.69 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 20 | 0.69 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 12 | 0.69 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 15 | 0.69 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 15 | 0.69 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 15 | 0.69 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 2 | 0.69 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 2 | 0.69 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 2 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 9 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 9 | 0.69 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 9 | 0.69 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 1 | 0.69 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 1 | 0.69 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 16 | 0.69 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 16 | 0.69 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 19 | 0.69 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 19 | 0.69 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 18 | 0.69 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 18 | 0.69 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 18 | 0.69 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 10 | 0.69 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 10 | 0.69 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 20 | 0.69 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 10 | 0.69 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 10 | 0.69 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 10 | 0.69 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 13 | 0.69 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 13 | 0.69 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 13 | 0.69 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 8 | 0.69 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 8 | 0.69 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 8 | 0.69 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 8 | 0.69 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 8 | 0.69 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 8 | 0.69 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 8 | 0.69 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 8 | 0.69 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 7 | 0.69 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 7 | 0.69 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 7 | 0.69 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 1 | 0.69 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 1 | 0.69 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 1 | 0.69 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 14 | 0.69 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 1 | 0.69 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 1 | 0.69 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 1 | 0.69 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 1 | 0.69 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 1 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 1 | 0.69 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 17 | 0.69 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 17 | 0.69 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 17 | 0.69 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 17 | 0.69 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 17 | 0.69 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 17 | 0.69 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 4 | 0.69 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 4 | 0.69 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 4 | 0.69 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 12 | 0.69 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 12 | 0.69 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 12 | 0.69 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 1 | 0.69 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 6 | 0.69 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 6 | 0.69 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 6 | 0.69 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 5 | 0.69 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 5 | 0.69 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 5 | 0.69 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 6 | 0.69 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 6 | 0.69 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 6 | 0.69 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 15 | 0.68 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 15 | 0.68 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 15 | 0.68 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 15 | 0.68 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 15 | 0.68 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 15 | 0.68 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 3 | 0.68 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 3 | 0.68 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 3 | 0.68 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 3 | 0.68 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 3 | 0.68 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 3 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 11 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 11 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 15 | 0.68 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 15 | 0.68 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 17 | 0.68 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 17 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HG2 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HG3 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HG2 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HG3 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HG2 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HG3 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HG2 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HG3 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HG2 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HG3 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HG2 | 5 | 0.68 |
| (1,3663) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HG3 | 5 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG21 | 10 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG22 | 10 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG23 | 10 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG21 | 10 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG22 | 10 | 0.68 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG23 | 10 | 0.68 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 16 | 0.68 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 3 | 0.68 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 16 | 0.68 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 16 | 0.68 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 18 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 18 | 0.68 |
| (1,3280) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HA | 19 | 0.68 |
| (1,3280) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HA | 19 | 0.68 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 20 | 0.68 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 20 | 0.68 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 20 | 0.68 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 20 | 0.68 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 20 | 0.68 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 20 | 0.68 |
| (1,3074) | 1:167:A:ASP:H | 1:196:A:ASN:HD22 | 4 | 0.68 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 8 | 0.68 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 8 | 0.68 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 17 | 0.68 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 19 | 0.68 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 5 | 0.68 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 5 | 0.68 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 5 | 0.68 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 1 | 0.68 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 1 | 0.68 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 1 | 0.68 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 10 | 0.68 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 16 | 0.68 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 17 | 0.68 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 20 | 0.68 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 11 | 0.68 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 11 | 0.68 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 11 | 0.68 |
| (1,2375) | 1:92:A:LYS:HG2 | 1:93:A:GLU:H | 10 | 0.68 |
| (1,2375) | 1:92:A:LYS:HG3 | 1:93:A:GLU:H | 10 | 0.68 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 2 | 0.68 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 15 | 0.68 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 14 | 0.68 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD11 | 4 | 0.68 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD12 | 4 | 0.68 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD13 | 4 | 0.68 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 13 | 0.68 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 5 | 0.68 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 5 | 0.68 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 5 | 0.68 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 7 | 0.68 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 7 | 0.68 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 7 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 10 | 0.68 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 10 | 0.68 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 10 | 0.68 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 15 | 0.68 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 18 | 0.68 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 3 | 0.68 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 3 | 0.68 |
| (1,1731) | 1:167:A:ASP:HA | 1:196:A:ASN:HB3 | 19 | 0.68 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 5 | 0.68 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 5 | 0.68 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 5 | 0.68 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 18 | 0.68 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 18 | 0.68 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 18 | 0.68 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 5 | 0.68 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 5 | 0.68 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 5 | 0.68 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 20 | 0.68 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 20 | 0.68 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 20 | 0.68 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 18 | 0.68 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE2 | 9 | 0.68 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE3 | 9 | 0.68 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE2 | 9 | 0.68 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE3 | 9 | 0.68 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 6 | 0.68 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 6 | 0.68 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 5 | 0.68 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 7 | 0.68 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 7 | 0.68 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 7 | 0.68 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 9 | 0.68 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 2 | 0.68 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 2 | 0.68 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 2 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 19 | 0.68 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 19 | 0.68 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 19 | 0.68 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 19 | 0.68 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 19 | 0.68 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 19 | 0.68 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 19 | 0.68 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 9 | 0.68 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 9 | 0.68 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 9 | 0.68 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 14 | 0.68 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 13 | 0.68 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 13 | 0.68 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 13 | 0.68 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 12 | 0.68 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 20 | 0.68 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 17 | 0.68 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 17 | 0.68 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 6 | 0.68 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 6 | 0.68 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 6 | 0.68 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 6 | 0.68 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 6 | 0.68 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 6 | 0.68 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 16 | 0.68 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 16 | 0.68 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 16 | 0.68 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 16 | 0.68 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 16 | 0.68 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 16 | 0.68 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 8 | 0.68 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 8 | 0.68 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 8 | 0.68 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 5 | 0.68 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 17 | 0.68 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 18 | 0.68 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 18 | 0.68 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 9 | 0.68 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 9 | 0.68 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 4 | 0.68 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 4 | 0.68 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 4 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 2 | 0.68 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 2 | 0.68 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 2 | 0.68 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 19 | 0.68 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 19 | 0.68 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 5 | 0.68 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 18 | 0.68 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 18 | 0.68 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 18 | 0.68 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 18 | 0.68 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 18 | 0.68 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 18 | 0.68 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 9 | 0.68 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD11 | 13 | 0.68 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD12 | 13 | 0.68 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD13 | 13 | 0.68 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 3 | 0.68 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 3 | 0.68 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 3 | 0.68 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 2 | 0.68 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 2 | 0.68 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 2 | 0.68 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 11 | 0.67 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 11 | 0.67 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 11 | 0.67 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 11 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 18 | 0.67 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 18 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 15 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 15 | 0.67 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 15 | 0.67 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 9 | 0.67 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 9 | 0.67 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 7 | 0.67 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 7 | 0.67 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 5 | 0.67 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 5 | 0.67 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 5 | 0.67 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 5 | 0.67 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 5 | 0.67 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 5 | 0.67 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 7 | 0.67 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 7 | 0.67 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 7 | 0.67 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 10 | 0.67 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 10 | 0.67 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 2 | 0.67 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 11 | 0.67 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 11 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 4 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 4 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 10 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 10 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 17 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 17 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 18 | 0.67 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 18 | 0.67 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 1 | 0.67 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 1 | 0.67 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 1 | 0.67 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 1 | 0.67 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 1 | 0.67 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 1 | 0.67 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 18 | 0.67 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 19 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 2 | 0.67 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 13 | 0.67 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 12 | 0.67 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 2 | 0.67 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 2 | 0.67 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 3 | 0.67 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 3 | 0.67 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 3 | 0.67 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 6 | 0.67 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 6 | 0.67 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 6 | 0.67 |
| (1,2638) | 1:142:A:THR:HG21 | 1:147:A:GLY:H | 12 | 0.67 |
| (1,2638) | 1:142:A:THR:HG22 | 1:147:A:GLY:H | 12 | 0.67 |
| (1,2638) | 1:142:A:THR:HG23 | 1:147:A:GLY:H | 12 | 0.67 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 6 | 0.67 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 6 | 0.67 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 6 | 0.67 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 12 | 0.67 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 2 | 0.67 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 11 | 0.67 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 20 | 0.67 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 20 | 0.67 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 9 | 0.67 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 9 | 0.67 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 9 | 0.67 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 19 | 0.67 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 5 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 6 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 6 | 0.67 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 6 | 0.67 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 12 | 0.67 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 12 | 0.67 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 19 | 0.67 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 19 | 0.67 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 11 | 0.67 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 11 | 0.67 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 11 | 0.67 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 1 | 0.67 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 10 | 0.67 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 10 | 0.67 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 10 | 0.67 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 13 | 0.67 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 20 | 0.67 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 20 | 0.67 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 20 | 0.67 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 20 | 0.67 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 20 | 0.67 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 20 | 0.67 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 4 | 0.67 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 4 | 0.67 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 4 | 0.67 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 8 | 0.67 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 18 | 0.67 |
| (1,780) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG12 | 5 | 0.67 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 4 | 0.67 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 4 | 0.67 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 4 | 0.67 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 10 | 0.67 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 7 | 0.67 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 7 | 0.67 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 3 | 0.67 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 3 | 0.67 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 3 | 0.67 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 3 | 0.67 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 3 | 0.67 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 3 | 0.67 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 9 | 0.67 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 9 | 0.67 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 9 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 9 | 0.67 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 9 | 0.67 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 9 | 0.67 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 12 | 0.67 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 12 | 0.67 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 12 | 0.67 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 12 | 0.67 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 12 | 0.67 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 12 | 0.67 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 2 | 0.67 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 2 | 0.67 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 2 | 0.67 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 2 | 0.67 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 2 | 0.67 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 2 | 0.67 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 2 | 0.67 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 2 | 0.67 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 2 | 0.67 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 4 | 0.67 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 4 | 0.67 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 4 | 0.67 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 9 | 0.67 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 9 | 0.67 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 9 | 0.67 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 14 | 0.67 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 14 | 0.67 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 14 | 0.67 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 7 | 0.67 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 7 | 0.67 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 7 | 0.67 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 1 | 0.67 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 1 | 0.67 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 1 | 0.67 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 1 | 0.67 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 1 | 0.67 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 1 | 0.67 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 20 | 0.67 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 16 | 0.67 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 16 | 0.67 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 16 | 0.67 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 15 | 0.67 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 15 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 15 | 0.67 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 4 | 0.67 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 17 | 0.67 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 6 | 0.67 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 3 | 0.67 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 3 | 0.67 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 3 | 0.67 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 5 | 0.67 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 5 | 0.67 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 5 | 0.67 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD11 | 6 | 0.67 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD12 | 6 | 0.67 |
| (1,7) | 1:47:A:THR:HA | 1:50:A:LEU:HD13 | 6 | 0.67 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 8 | 0.67 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 8 | 0.67 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 2 | 0.66 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 2 | 0.66 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 18 | 0.66 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 18 | 0.66 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 13 | 0.66 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 13 | 0.66 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 16 | 0.66 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 16 | 0.66 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 16 | 0.66 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 16 | 0.66 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 16 | 0.66 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 16 | 0.66 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 15 | 0.66 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 15 | 0.66 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 15 | 0.66 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 15 | 0.66 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 19 | 0.66 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 19 | 0.66 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 14 | 0.66 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 14 | 0.66 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 5 | 0.66 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 5 | 0.66 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 5 | 0.66 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 5 | 0.66 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 5 | 0.66 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 5 | 0.66 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 2 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 2 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE1 | 4 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE2 | 4 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE3 | 4 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE1 | 4 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE2 | 4 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE3 | 4 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE1 | 6 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE2 | 6 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE1 | 2:21:B:MET:HE3 | 6 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE1 | 6 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE2 | 6 | 0.66 |
| (1,3531) | 1:63:A:TYR:HE2 | 2:21:B:MET:HE3 | 6 | 0.66 |
| (1,3506) | 1:51:A:PRO:HB3 | 2:7:B:PRO:HD2 | 12 | 0.66 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 10 | 0.66 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 10 | 0.66 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 10 | 0.66 |
| (1,3370) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG2 | 14 | 0.66 |
| (1,3370) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG2 | 14 | 0.66 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 7 | 0.66 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 7 | 0.66 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 7 | 0.66 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 7 | 0.66 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 5 | 0.66 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 2 | 0.66 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 17 | 0.66 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 16 | 0.66 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 12 | 0.66 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 17 | 0.66 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 16 | 0.66 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 12 | 0.66 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 18 | 0.66 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 18 | 0.66 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 18 | 0.66 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 17 | 0.66 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 20 | 0.66 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 14 | 0.66 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 14 | 0.66 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 14 | 0.66 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 2 | 0.66 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 1 | 0.66 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 2 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 14 | 0.66 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 5 | 0.66 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 5 | 0.66 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 5 | 0.66 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 3 | 0.66 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 6 | 0.66 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 4 | 0.66 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 4 | 0.66 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 4 | 0.66 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 4 | 0.66 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 4 | 0.66 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 4 | 0.66 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 8 | 0.66 |
| (1,1696) | 1:194:A:ILE:HD11 | 1:221:A:THR:HB | 1 | 0.66 |
| (1,1696) | 1:194:A:ILE:HD12 | 1:221:A:THR:HB | 1 | 0.66 |
| (1,1696) | 1:194:A:ILE:HD13 | 1:221:A:THR:HB | 1 | 0.66 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 20 | 0.66 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 20 | 0.66 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 20 | 0.66 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 8 | 0.66 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 8 | 0.66 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 8 | 0.66 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 6 | 0.66 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 6 | 0.66 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 6 | 0.66 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 15 | 0.66 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 15 | 0.66 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 15 | 0.66 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 1 | 0.66 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 1 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 11 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 11 | 0.66 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 11 | 0.66 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 17 | 0.66 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 17 | 0.66 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 17 | 0.66 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 20 | 0.66 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 20 | 0.66 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 18 | 0.66 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 4 | 0.66 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 4 | 0.66 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 4 | 0.66 |
| (1,1098) | 1:139:A:SER:HB2 | 1:140:A:ILE:HG21 | 12 | 0.66 |
| (1,1098) | 1:139:A:SER:HB2 | 1:140:A:ILE:HG22 | 12 | 0.66 |
| (1,1098) | 1:139:A:SER:HB2 | 1:140:A:ILE:HG23 | 12 | 0.66 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 15 | 0.66 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 15 | 0.66 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 16 | 0.66 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 16 | 0.66 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 16 | 0.66 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 16 | 0.66 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 16 | 0.66 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 16 | 0.66 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 5 | 0.66 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 5 | 0.66 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 5 | 0.66 |
| (1,676) | 1:103:A:THR:HG21 | 1:128:A:LEU:H | 20 | 0.66 |
| (1,676) | 1:103:A:THR:HG22 | 1:128:A:LEU:H | 20 | 0.66 |
| (1,676) | 1:103:A:THR:HG23 | 1:128:A:LEU:H | 20 | 0.66 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 3 | 0.66 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 3 | 0.66 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 3 | 0.66 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 4 | 0.66 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 4 | 0.66 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 4 | 0.66 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 4 | 0.66 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 4 | 0.66 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 4 | 0.66 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 17 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 17 | 0.66 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 17 | 0.66 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 8 | 0.66 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 8 | 0.66 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 8 | 0.66 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 11 | 0.66 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 11 | 0.66 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 11 | 0.66 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 16 | 0.66 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 16 | 0.66 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 16 | 0.66 |
| (1,314) | 1:70:A:THR:HG21 | 1:86:A:GLU:HG2 | 18 | 0.66 |
| (1,314) | 1:70:A:THR:HG22 | 1:86:A:GLU:HG2 | 18 | 0.66 |
| (1,314) | 1:70:A:THR:HG23 | 1:86:A:GLU:HG2 | 18 | 0.66 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 4 | 0.66 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 4 | 0.66 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 4 | 0.66 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 7 | 0.66 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 13 | 0.66 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 18 | 0.66 |
| (1,12) | 1:47:A:THR:HB | 1:50:A:LEU:HG | 20 | 0.66 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 5 | 0.66 |
| (1,4003) | 2:8:B:ILE:HD11 | 2:21:B:MET:HG2 | 2 | 0.65 |
| (1,4003) | 2:8:B:ILE:HD11 | 2:21:B:MET:HG3 | 2 | 0.65 |
| (1,4003) | 2:8:B:ILE:HD12 | 2:21:B:MET:HG2 | 2 | 0.65 |
| (1,4003) | 2:8:B:ILE:HD12 | 2:21:B:MET:HG3 | 2 | 0.65 |
| (1,4003) | 2:8:B:ILE:HD13 | 2:21:B:MET:HG2 | 2 | 0.65 |
| (1,4003) | 2:8:B:ILE:HD13 | 2:21:B:MET:HG3 | 2 | 0.65 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 12 | 0.65 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 12 | 0.65 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 12 | 0.65 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 12 | 0.65 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 12 | 0.65 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 12 | 0.65 |
| (1,3635) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE21 | 4 | 0.65 |
| (1,3635) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 4 | 0.65 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 4 | 0.65 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 4 | 0.65 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 4 | 0.65 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 4 | 0.65 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 4 | 0.65 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 4 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 19 | 0.65 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 19 | 0.65 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 13 | 0.65 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 13 | 0.65 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 16 | 0.65 |
| (1,3235) | 1:125:A:TRP:HZ3 | 1:155:A:LYS:HB3 | 9 | 0.65 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 7 | 0.65 |
| (1,3055) | 1:193:A:THR:HG21 | 1:195:A:ASN:HD21 | 2 | 0.65 |
| (1,3055) | 1:193:A:THR:HG22 | 1:195:A:ASN:HD21 | 2 | 0.65 |
| (1,3055) | 1:193:A:THR:HG23 | 1:195:A:ASN:HD21 | 2 | 0.65 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 15 | 0.65 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 19 | 0.65 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 15 | 0.65 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 13 | 0.65 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 11 | 0.65 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 3 | 0.65 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 6 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 10 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 10 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 10 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 11 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 11 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 11 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 12 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 12 | 0.65 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 12 | 0.65 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 9 | 0.65 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 9 | 0.65 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 9 | 0.65 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 9 | 0.65 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 9 | 0.65 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 9 | 0.65 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 9 | 0.65 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 9 | 0.65 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 9 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 3 | 0.65 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 3 | 0.65 |
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 18 | 0.65 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 10 | 0.65 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 10 | 0.65 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 10 | 0.65 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 14 | 0.65 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 14 | 0.65 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 14 | 0.65 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 19 | 0.65 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 19 | 0.65 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 19 | 0.65 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 9 | 0.65 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 9 | 0.65 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 9 | 0.65 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 2 | 0.65 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 19 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 7 | 0.65 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 7 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 15 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 15 | 0.65 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 15 | 0.65 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 7 | 0.65 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 13 | 0.65 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 13 | 0.65 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 4 | 0.65 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 15 | 0.65 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 15 | 0.65 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 15 | 0.65 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 16 | 0.65 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 16 | 0.65 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 16 | 0.65 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 5 | 0.65 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 18 | 0.65 |
| (1,1149) | 1:148:A:SER:HA | 1:179:A:LEU:HD11 | 19 | 0.65 |
| (1,1149) | 1:148:A:SER:HA | 1:179:A:LEU:HD12 | 19 | 0.65 |
| (1,1149) | 1:148:A:SER:HA | 1:179:A:LEU:HD13 | 19 | 0.65 |
| (1,1149) | 1:148:A:SER:HA | 1:179:A:LEU:HD21 | 19 | 0.65 |
| (1,1149) | 1:148:A:SER:HA | 1:179:A:LEU:HD22 | 19 | 0.65 |
| (1,1149) | 1:148:A:SER:HA | 1:179:A:LEU:HD23 | 19 | 0.65 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 20 | 0.65 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 10 | 0.65 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 10 | 0.65 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 10 | 0.65 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 18 | 0.65 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 18 | 0.65 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 18 | 0.65 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 20 | 0.65 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 20 | 0.65 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 20 | 0.65 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 7 | 0.65 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 9 | 0.65 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 9 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 13 | 0.65 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 13 | 0.65 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 13 | 0.65 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 10 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 4 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 4 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 4 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 19 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 19 | 0.65 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 19 | 0.65 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 16 | 0.65 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 16 | 0.65 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 16 | 0.65 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 11 | 0.65 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 11 | 0.65 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 11 | 0.65 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 13 | 0.65 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 13 | 0.65 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 7 | 0.65 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 7 | 0.65 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 7 | 0.65 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 7 | 0.65 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 16 | 0.65 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 17 | 0.65 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 12 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 12 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 12 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 12 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 12 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 12 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 17 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 17 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 17 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 17 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 17 | 0.64 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 17 | 0.64 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 5 | 0.64 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 5 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 19 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 19 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 19 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 19 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 19 | 0.64 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 19 | 0.64 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 1 | 0.64 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 1 | 0.64 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 1 | 0.64 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 1 | 0.64 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 15 | 0.64 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 15 | 0.64 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 15 | 0.64 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 15 | 0.64 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 15 | 0.64 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 15 | 0.64 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 18 | 0.64 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 18 | 0.64 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 15 | 0.64 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 15 | 0.64 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 7 | 0.64 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 7 | 0.64 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 3 | 0.64 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 18 | 0.64 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 3 | 0.64 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 3 | 0.64 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 18 | 0.64 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 18 | 0.64 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 18 | 0.64 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 18 | 0.64 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 18 | 0.64 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 18 | 0.64 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 5 | 0.64 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 5 | 0.64 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 5 | 0.64 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 16 | 0.64 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 16 | 0.64 |
| (1,2941) | 1:196:A:ASN:HD21 | 1:197:A:ALA:H | 9 | 0.64 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 14 | 0.64 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 14 | 0.64 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 14 | 0.64 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 7 | 0.64 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 16 | 0.64 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 4 | 0.64 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 8 | 0.64 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 13 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 14 | 0.64 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 17 | 0.64 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 9 | 0.64 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 1 | 0.64 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 1 | 0.64 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 1 | 0.64 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 16 | 0.64 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 16 | 0.64 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 16 | 0.64 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 15 | 0.64 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 15 | 0.64 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 15 | 0.64 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 14 | 0.64 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 1 | 0.64 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 1 | 0.64 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 1 | 0.64 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 6 | 0.64 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 6 | 0.64 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 6 | 0.64 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 11 | 0.64 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 11 | 0.64 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 11 | 0.64 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 18 | 0.64 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 18 | 0.64 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 18 | 0.64 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 9 | 0.64 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 9 | 0.64 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 9 | 0.64 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 9 | 0.64 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 9 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 4 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 4 | 0.64 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 4 | 0.64 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 4 | 0.64 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 8 | 0.64 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 8 | 0.64 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 1 | 0.64 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 1 | 0.64 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 15 | 0.64 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 15 | 0.64 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 9 | 0.64 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 9 | 0.64 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 9 | 0.64 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 12 | 0.64 |
| (1,1256) | 1:155:A:LYS:HE3 | 1:156:A:SER:H | 16 | 0.64 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 13 | 0.64 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 13 | 0.64 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 13 | 0.64 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 11 | 0.64 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 8 | 0.64 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 15 | 0.64 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 15 | 0.64 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 15 | 0.64 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 15 | 0.64 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 15 | 0.64 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 15 | 0.64 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD21 | 9 | 0.64 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD22 | 9 | 0.64 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD23 | 9 | 0.64 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 8 | 0.64 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 8 | 0.64 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 8 | 0.64 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 1 | 0.64 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 1 | 0.64 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 1 | 0.64 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 5 | 0.64 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 14 | 0.64 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 14 | 0.64 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 14 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 14 | 0.64 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 14 | 0.64 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 14 | 0.64 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 7 | 0.64 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 7 | 0.64 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 7 | 0.64 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 7 | 0.64 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 6 | 0.64 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 6 | 0.64 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 6 | 0.64 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 5 | 0.64 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 5 | 0.64 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 5 | 0.64 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 17 | 0.64 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 17 | 0.64 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 17 | 0.64 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 6 | 0.64 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 4 | 0.64 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 4 | 0.64 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 4 | 0.64 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 4 | 0.64 |
| (1,232) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 17 | 0.64 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 19 | 0.64 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 18 | 0.64 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 16 | 0.64 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 16 | 0.64 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 16 | 0.64 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG2 | 7 | 0.63 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG3 | 7 | 0.63 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG2 | 7 | 0.63 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG3 | 7 | 0.63 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG2 | 7 | 0.63 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG3 | 7 | 0.63 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 13 | 0.63 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 13 | 0.63 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 13 | 0.63 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 13 | 0.63 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 13 | 0.63 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 13 | 0.63 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 13 | 0.63 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 13 | 0.63 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 13 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 13 | 0.63 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 13 | 0.63 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 13 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 7 | 0.63 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 7 | 0.63 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD2 | 15 | 0.63 |
| (1,3594) | 1:76:A:MET:HA | 1:81:A:ARG:HD3 | 15 | 0.63 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 11 | 0.63 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 11 | 0.63 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 14 | 0.63 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 14 | 0.63 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 6 | 0.63 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 6 | 0.63 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 6 | 0.63 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 6 | 0.63 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 6 | 0.63 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 6 | 0.63 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 12 | 0.63 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 12 | 0.63 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 13 | 0.63 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 13 | 0.63 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 13 | 0.63 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 13 | 0.63 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 13 | 0.63 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 13 | 0.63 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 13 | 0.63 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 13 | 0.63 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 5 | 0.63 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 5 | 0.63 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 5 | 0.63 |
| (1,3401) | 2:6:B:VAL:HG21 | 2:7:B:PRO:HD3 | 1 | 0.63 |
| (1,3401) | 2:6:B:VAL:HG22 | 2:7:B:PRO:HD3 | 1 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3401) | 2:6:B:VAL:HG23 | 2:7:B:PRO:HD3 | 1 | 0.63 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 16 | 0.63 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 16 | 0.63 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 14 | 0.63 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 14 | 0.63 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 3 | 0.63 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 10 | 0.63 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 7 | 0.63 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 13 | 0.63 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 13 | 0.63 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 13 | 0.63 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 18 | 0.63 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 18 | 0.63 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 2 | 0.63 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 2 | 0.63 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 2 | 0.63 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 17 | 0.63 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 17 | 0.63 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 17 | 0.63 |
| (1,2651) | 1:141:A:GLU:HG2 | 1:149:A:ALA:H | 7 | 0.63 |
| (1,2651) | 1:141:A:GLU:HG3 | 1:149:A:ALA:H | 7 | 0.63 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 8 | 0.63 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 13 | 0.63 |
| (1,2303) | 1:77:A:GLN:HB2 | 1:80:A:SER:H | 10 | 0.63 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 14 | 0.63 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 15 | 0.63 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 13 | 0.63 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 13 | 0.63 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 13 | 0.63 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 10 | 0.63 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 3 | 0.63 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 3 | 0.63 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 3 | 0.63 |
| (1,1963) | 1:161:A:LYS:HD2 | 1:189:A:VAL:H | 9 | 0.63 |
| (1,1963) | 1:161:A:LYS:HD3 | 1:189:A:VAL:H | 9 | 0.63 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 13 | 0.63 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 14 | 0.63 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 14 | 0.63 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 14 | 0.63 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 19 | 0.63 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 19 | 0.63 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 19 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1732) | 1:196:A:ASN:HB2 | 1:225:A:LYS:HB3 | 15 | 0.63 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 9 | 0.63 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 9 | 0.63 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 9 | 0.63 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 18 | 0.63 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 18 | 0.63 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 18 | 0.63 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 3 | 0.63 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 3 | 0.63 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 3 | 0.63 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 16 | 0.63 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 16 | 0.63 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 16 | 0.63 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 3 | 0.63 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 3 | 0.63 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 3 | 0.63 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 3 | 0.63 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 10 | 0.63 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 20 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 1 | 0.63 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 1 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 18 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 18 | 0.63 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 18 | 0.63 |
| (1,1383) | 1:169:A:THR:HG21 | 1:171:A:ASP:HA | 3 | 0.63 |
| (1,1383) | 1:169:A:THR:HG22 | 1:171:A:ASP:HA | 3 | 0.63 |
| (1,1383) | 1:169:A:THR:HG23 | 1:171:A:ASP:HA | 3 | 0.63 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 3 | 0.63 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 5 | 0.63 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 5 | 0.63 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 14 | 0.63 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 14 | 0.63 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 20 | 0.63 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 20 | 0.63 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 11 | 0.63 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 11 | 0.63 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 2 | 0.63 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 2 | 0.63 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 2 | 0.63 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 20 | 0.63 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 13 | 0.63 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 13 | 0.63 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 13 | 0.63 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 9 | 0.63 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 9 | 0.63 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 8 | 0.63 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 8 | 0.63 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 8 | 0.63 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 3 | 0.63 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 17 | 0.63 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 13 | 0.63 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 17 | 0.63 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 17 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 17 | 0.63 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 3 | 0.63 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 16 | 0.63 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 15 | 0.63 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 15 | 0.63 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 15 | 0.63 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 15 | 0.63 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 15 | 0.63 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 15 | 0.63 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 10 | 0.63 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 11 | 0.63 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 11 | 0.63 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 20 | 0.63 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 7 | 0.63 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 7 | 0.63 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 7 | 0.63 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 10 | 0.63 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 10 | 0.63 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 10 | 0.63 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 14 | 0.63 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 14 | 0.63 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 14 | 0.63 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 15 | 0.63 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 15 | 0.63 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 15 | 0.63 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 16 | 0.63 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 16 | 0.63 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 16 | 0.63 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 14 | 0.63 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 3 | 0.63 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 3 | 0.63 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 3 | 0.63 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 18 | 0.63 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 18 | 0.63 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 18 | 0.63 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 18 | 0.63 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 18 | 0.63 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 18 | 0.63 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 15 | 0.63 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 15 | 0.63 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 13 | 0.62 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 13 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 8 | 0.62 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 8 | 0.62 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 8 | 0.62 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 8 | 0.62 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 8 | 0.62 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 8 | 0.62 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 15 | 0.62 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 15 | 0.62 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 15 | 0.62 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 15 | 0.62 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 15 | 0.62 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 15 | 0.62 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 19 | 0.62 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 19 | 0.62 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 19 | 0.62 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 19 | 0.62 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 19 | 0.62 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 19 | 0.62 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB2 | 7 | 0.62 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB3 | 7 | 0.62 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB2 | 7 | 0.62 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB3 | 7 | 0.62 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB2 | 7 | 0.62 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB3 | 7 | 0.62 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 14 | 0.62 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 14 | 0.62 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 18 | 0.62 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 18 | 0.62 |
| (1,3488) | 1:54:A:ILE:HD11 | 2:11:B:CYS:H | 16 | 0.62 |
| (1,3488) | 1:54:A:ILE:HD12 | 2:11:B:CYS:H | 16 | 0.62 |
| (1,3488) | 1:54:A:ILE:HD13 | 2:11:B:CYS:H | 16 | 0.62 |
| (1,3479) | 1:53:A:THR:HG21 | 2:9:B:ILE:HB | 3 | 0.62 |
| (1,3479) | 1:53:A:THR:HG22 | 2:9:B:ILE:HB | 3 | 0.62 |
| (1,3479) | 1:53:A:THR:HG23 | 2:9:B:ILE:HB | 3 | 0.62 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 15 | 0.62 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 15 | 0.62 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 15 | 0.62 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 4 | 0.62 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 4 | 0.62 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 4 | 0.62 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 4 | 0.62 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 4 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 4 | 0.62 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 20 | 0.62 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 20 | 0.62 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 12 | 0.62 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 12 | 0.62 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 12 | 0.62 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 7 | 0.62 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 7 | 0.62 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 7 | 0.62 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 6 | 0.62 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 15 | 0.62 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 15 | 0.62 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 15 | 0.62 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 15 | 0.62 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 15 | 0.62 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 15 | 0.62 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 1 | 0.62 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 4 | 0.62 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 4 | 0.62 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 4 | 0.62 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 1 | 0.62 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 1 | 0.62 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 12 | 0.62 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 12 | 0.62 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 13 | 0.62 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 13 | 0.62 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 5 | 0.62 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 4 | 0.62 |
| (1,2139) | 1:48:A:ASN:H | 1:49:A:ASP:H | 6 | 0.62 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 17 | 0.62 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 17 | 0.62 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 17 | 0.62 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 4 | 0.62 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 4 | 0.62 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 4 | 0.62 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 14 | 0.62 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 9 | 0.62 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 9 | 0.62 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 9 | 0.62 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 2 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 13 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 13 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 13 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 20 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 20 | 0.62 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 20 | 0.62 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 13 | 0.62 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 13 | 0.62 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 13 | 0.62 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 9 | 0.62 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 9 | 0.62 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 9 | 0.62 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 9 | 0.62 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 9 | 0.62 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 9 | 0.62 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 9 | 0.62 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 9 | 0.62 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 9 | 0.62 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 10 | 0.62 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 10 | 0.62 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 10 | 0.62 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 12 | 0.62 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 12 | 0.62 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 12 | 0.62 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 12 | 0.62 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 12 | 0.62 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 12 | 0.62 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 19 | 0.62 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 13 | 0.62 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 13 | 0.62 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 13 | 0.62 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 19 | 0.62 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 19 | 0.62 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 19 | 0.62 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 15 | 0.62 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 15 | 0.62 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 15 | 0.62 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 6 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 8 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 8 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 10 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 14 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 14 | 0.62 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 14 | 0.62 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 6 | 0.62 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 6 | 0.62 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 9 | 0.62 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 17 | 0.62 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 8 | 0.62 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 8 | 0.62 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 8 | 0.62 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 5 | 0.62 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 17 | 0.62 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 17 | 0.62 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 12 | 0.62 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 7 | 0.62 |
| (1,956) | 1:190:A:LYS:HA | 1:190:A:LYS:HE3 | 5 | 0.62 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 9 | 0.62 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 9 | 0.62 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 9 | 0.62 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 20 | 0.62 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 20 | 0.62 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 6 | 0.62 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 6 | 0.62 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 6 | 0.62 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG11 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG12 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG13 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG21 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG22 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG23 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG11 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG12 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG13 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG21 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG22 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG23 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG11 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG12 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG13 | 7 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG21 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG22 | 7 | 0.62 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG23 | 7 | 0.62 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 4 | 0.62 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 4 | 0.62 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 4 | 0.62 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 7 | 0.62 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 7 | 0.62 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 7 | 0.62 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 9 | 0.62 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 9 | 0.62 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 9 | 0.62 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 2 | 0.62 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 3 | 0.62 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 3 | 0.62 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 3 | 0.62 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 5 | 0.62 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 5 | 0.62 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 5 | 0.62 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 16 | 0.62 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 16 | 0.62 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 16 | 0.62 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 2 | 0.62 |
| (1,329) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HA | 3 | 0.62 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 11 | 0.62 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 13 | 0.62 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 13 | 0.62 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 20 | 0.62 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 1 | 0.61 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 1 | 0.61 |
| (1,3547) | 1:52:A:VAL:HG11 | 1:77:A:GLN:HG2 | 6 | 0.61 |
| (1,3547) | 1:52:A:VAL:HG11 | 1:77:A:GLN:HG3 | 6 | 0.61 |
| (1,3547) | 1:52:A:VAL:HG12 | 1:77:A:GLN:HG2 | 6 | 0.61 |
| (1,3547) | 1:52:A:VAL:HG12 | 1:77:A:GLN:HG3 | 6 | 0.61 |
| (1,3547) | 1:52:A:VAL:HG13 | 1:77:A:GLN:HG2 | 6 | 0.61 |
| (1,3547) | 1:52:A:VAL:HG13 | 1:77:A:GLN:HG3 | 6 | 0.61 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 6 | 0.61 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 6 | 0.61 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 6 | 0.61 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 6 | 0.61 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 4 | 0.61 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 4 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 4 | 0.61 |
| (1,3079) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 20 | 0.61 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 3 | 0.61 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 17 | 0.61 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 17 | 0.61 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 10 | 0.61 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 7 | 0.61 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 7 | 0.61 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 17 | 0.61 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 2 | 0.61 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 10 | 0.61 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 10 | 0.61 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 11 | 0.61 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 11 | 0.61 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 11 | 0.61 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 4 | 0.61 |
| (1,1878) | 1:202:A:THR:HA | 1:205:A:LYS:HG3 | 5 | 0.61 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 17 | 0.61 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 17 | 0.61 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 17 | 0.61 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE2 | 2 | 0.61 |
| (1,1833) | 1:202:A:THR:HG21 | 1:205:A:LYS:HE3 | 2 | 0.61 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE2 | 2 | 0.61 |
| (1,1833) | 1:202:A:THR:HG22 | 1:205:A:LYS:HE3 | 2 | 0.61 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE2 | 2 | 0.61 |
| (1,1833) | 1:202:A:THR:HG23 | 1:205:A:LYS:HE3 | 2 | 0.61 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 19 | 0.61 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 19 | 0.61 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 15 | 0.61 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 15 | 0.61 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 15 | 0.61 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 16 | 0.61 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 16 | 0.61 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 16 | 0.61 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 8 | 0.61 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 8 | 0.61 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 8 | 0.61 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 8 | 0.61 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 8 | 0.61 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 8 | 0.61 |
| (1,1611) | 1:116:A:GLN:HE21 | 1:187:A:MET:HA | 13 | 0.61 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 10 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 10 | 0.61 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 10 | 0.61 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 7 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 16 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 20 | 0.61 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 20 | 0.61 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 17 | 0.61 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 13 | 0.61 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 13 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 12 | 0.61 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 6 | 0.61 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 6 | 0.61 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 7 | 0.61 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 7 | 0.61 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 18 | 0.61 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 18 | 0.61 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 20 | 0.61 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 20 | 0.61 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 20 | 0.61 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 10 | 0.61 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 6 | 0.61 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 6 | 0.61 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 6 | 0.61 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 5 | 0.61 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 5 | 0.61 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 5 | 0.61 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 5 | 0.61 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 5 | 0.61 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 5 | 0.61 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 19 | 0.61 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 19 | 0.61 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 4 | 0.61 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 5 | 0.61 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 5 | 0.61 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 2 | 0.61 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 2 | 0.61 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 2 | 0.61 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 19 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 1 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 1 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 1 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 1 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 1 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 1 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 7 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 7 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 7 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 7 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 7 | 0.61 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 7 | 0.61 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 6 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 6 | 0.61 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 6 | 0.61 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB1 | 14 | 0.61 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB2 | 14 | 0.61 |
| (1,697) | 1:87:A:VAL:HB | 1:106:A:ALA:HB3 | 14 | 0.61 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 5 | 0.61 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 5 | 0.61 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 13 | 0.61 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 13 | 0.61 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 17 | 0.61 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 17 | 0.61 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 17 | 0.61 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 9 | 0.61 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 9 | 0.61 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 9 | 0.61 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 12 | 0.61 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 12 | 0.61 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 12 | 0.61 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 17 | 0.61 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 3 | 0.61 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 3 | 0.61 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 3 | 0.61 |
| (1,348) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HB2 | 16 | 0.61 |
| (1,348) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HB2 | 16 | 0.61 |
| (1,348) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HB2 | 16 | 0.61 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 7 | 0.61 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 7 | 0.61 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 19 | 0.61 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 19 | 0.61 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 19 | 0.61 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 18 | 0.61 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 18 | 0.61 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 18 | 0.61 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 2 | 0.61 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 7 | 0.61 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 10 | 0.61 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 15 | 0.61 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 15 | 0.61 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 15 | 0.61 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 9 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 9 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 9 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 9 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 9 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 9 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 16 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 16 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 16 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 16 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 16 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 16 | 0.6 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD11 | 5 | 0.6 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD12 | 5 | 0.6 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD13 | 5 | 0.6 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD21 | 5 | 0.6 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD22 | 5 | 0.6 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD23 | 5 | 0.6 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE2 | 12 | 0.6 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE3 | 12 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 14 | 0.6 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 14 | 0.6 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 4 | 0.6 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 4 | 0.6 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 4 | 0.6 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 4 | 0.6 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 4 | 0.6 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 4 | 0.6 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 7 | 0.6 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 7 | 0.6 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 7 | 0.6 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 7 | 0.6 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 7 | 0.6 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 7 | 0.6 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 4 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 14 | 0.6 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 14 | 0.6 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 15 | 0.6 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 15 | 0.6 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 8 | 0.6 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 8 | 0.6 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 8 | 0.6 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 16 | 0.6 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 16 | 0.6 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 12 | 0.6 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 12 | 0.6 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 14 | 0.6 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 9 | 0.6 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 15 | 0.6 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 15 | 0.6 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 1 | 0.6 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 13 | 0.6 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 2 | 0.6 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 8 | 0.6 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 17 | 0.6 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 18 | 0.6 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 5 | 0.6 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 5 | 0.6 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 10 | 0.6 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 10 | 0.6 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 5 | 0.6 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 5 | 0.6 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 5 | 0.6 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 15 | 0.6 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 15 | 0.6 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 15 | 0.6 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 3 | 0.6 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 9 | 0.6 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 16 | 0.6 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 4 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 4 | 0.6 |
| (1,2437) | 1:82:A:LEU:HG | 1:113:A:ASP:H | 10 | 0.6 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 1 | 0.6 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 12 | 0.6 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 14 | 0.6 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 10 | 0.6 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 10 | 0.6 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 10 | 0.6 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 5 | 0.6 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 14 | 0.6 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 11 | 0.6 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 11 | 0.6 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 14 | 0.6 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 18 | 0.6 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 14 | 0.6 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 1 | 0.6 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 1 | 0.6 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 1 | 0.6 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 18 | 0.6 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 18 | 0.6 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 18 | 0.6 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 9 | 0.6 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 6 | 0.6 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 6 | 0.6 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 6 | 0.6 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 4 | 0.6 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 4 | 0.6 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 4 | 0.6 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 1 | 0.6 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 1 | 0.6 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 1 | 0.6 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 3 | 0.6 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 9 | 0.6 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 9 | 0.6 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 11 | 0.6 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 11 | 0.6 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 6 | 0.6 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 16 | 0.6 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 13 | 0.6 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 1 | 0.6 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 1 | 0.6 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 1 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 12 | 0.6 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 15 | 0.6 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 2 | 0.6 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 9 | 0.6 |
| (1,956) | 1:190:A:LYS:HA | 1:190:A:LYS:HE3 | 16 | 0.6 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 1 | 0.6 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 9 | 0.6 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 9 | 0.6 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 9 | 0.6 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 19 | 0.6 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 19 | 0.6 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 19 | 0.6 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 19 | 0.6 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 15 | 0.6 |
| (1,693) | 1:84:A:ALA:HA | 1:106:A:ALA:HA | 4 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 8 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 8 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 8 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 11 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 11 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 11 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 15 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 15 | 0.6 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 15 | 0.6 |
| (1,541) | 1:94:A:ALA:H | 1:97:A:GLN:HG3 | 8 | 0.6 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 20 | 0.6 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 20 | 0.6 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 20 | 0.6 |
| (1,475) | 1:82:A:LEU:HA | 1:112:A:TYR:HD1 | 17 | 0.6 |
| (1,475) | 1:82:A:LEU:HA | 1:112:A:TYR:HD2 | 17 | 0.6 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 2 | 0.6 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 2 | 0.6 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 2 | 0.6 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 20 | 0.6 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 20 | 0.6 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 20 | 0.6 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 12 | 0.6 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 16 | 0.6 |
| (1,69) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE21 | 5 | 0.6 |
| (1,69) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE21 | 5 | 0.6 |
| (1,69) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE21 | 5 | 0.6 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 8 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 8 | 0.59 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 8 | 0.59 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 8 | 0.59 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 8 | 0.59 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 8 | 0.59 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 11 | 0.59 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 11 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 1 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 1 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 1 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 1 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 1 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 1 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 19 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 19 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 19 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 19 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 19 | 0.59 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 19 | 0.59 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 10 | 0.59 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 10 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 19 | 0.59 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 19 | 0.59 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 6 | 0.59 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 6 | 0.59 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 6 | 0.59 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 6 | 0.59 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 4 | 0.59 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 4 | 0.59 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 3 | 0.59 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 3 | 0.59 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 3 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 3 | 0.59 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 3 | 0.59 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 3 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 6 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 6 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 6 | 0.59 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 6 | 0.59 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 15 | 0.59 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 20 | 0.59 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 20 | 0.59 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 20 | 0.59 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 11 | 0.59 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 11 | 0.59 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 11 | 0.59 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 4 | 0.59 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 5 | 0.59 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 5 | 0.59 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 5 | 0.59 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 17 | 0.59 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 17 | 0.59 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 17 | 0.59 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 17 | 0.59 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 17 | 0.59 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 17 | 0.59 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 5 | 0.59 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 5 | 0.59 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 4 | 0.59 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 4 | 0.59 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 15 | 0.59 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 15 | 0.59 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 4 | 0.59 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 4 | 0.59 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 4 | 0.59 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 16 | 0.59 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 16 | 0.59 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 16 | 0.59 |
| (1,2765) | 1:168:A:ALA:H | 1:196:A:ASN:HA | 19 | 0.59 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 5 | 0.59 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 14 | 0.59 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 10 | 0.59 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 10 | 0.59 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 10 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 3 | 0.59 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 9 | 0.59 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 12 | 0.59 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE1 | 1 | 0.59 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE2 | 1 | 0.59 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 6 | 0.59 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 9 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 3 | 0.59 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 3 | 0.59 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 9 | 0.59 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 9 | 0.59 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 9 | 0.59 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 9 | 0.59 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 16 | 0.59 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 16 | 0.59 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 16 | 0.59 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 2 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 2 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 2 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 2 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 4 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 4 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 4 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 7 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 7 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 7 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 15 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 15 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 15 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 18 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 18 | 0.59 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 18 | 0.59 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 17 | 0.59 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 4 | 0.59 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 4 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 4 | 0.59 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 3 | 0.59 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 3 | 0.59 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 3 | 0.59 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 18 | 0.59 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 18 | 0.59 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 18 | 0.59 |
| (1,1485) | 1:177:A:GLU:HA | 1:180:A:ILE:HB | 14 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 12 | 0.59 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 12 | 0.59 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE2 | 4 | 0.59 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE3 | 4 | 0.59 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE2 | 4 | 0.59 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE3 | 4 | 0.59 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 3 | 0.59 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 3 | 0.59 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 4 | 0.59 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 4 | 0.59 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 8 | 0.59 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 15 | 0.59 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 15 | 0.59 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 15 | 0.59 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 9 | 0.59 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 9 | 0.59 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 9 | 0.59 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 14 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 14 | 0.59 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 14 | 0.59 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 5 | 0.59 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 5 | 0.59 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 14 | 0.59 |
| (1,999) | 1:136:A:TYR:HA | 1:152:A:LYS:HB2 | 10 | 0.59 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 3 | 0.59 |
| (1,956) | 1:190:A:LYS:HA | 1:190:A:LYS:HE3 | 20 | 0.59 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 4 | 0.59 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 1 | 0.59 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 1 | 0.59 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 1 | 0.59 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 5 | 0.59 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 4 | 0.59 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 4 | 0.59 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 4 | 0.59 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 7 | 0.59 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 7 | 0.59 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 7 | 0.59 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 11 | 0.59 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 11 | 0.59 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 11 | 0.59 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG11 | 13 | 0.59 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG12 | 13 | 0.59 |
| (1,787) | 1:115:A:ASN:HB2 | 1:143:A:VAL:HG13 | 13 | 0.59 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG11 | 13 | 0.59 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG12 | 13 | 0.59 |
| (1,787) | 1:115:A:ASN:HB3 | 1:143:A:VAL:HG13 | 13 | 0.59 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 1 | 0.59 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 10 | 0.59 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 10 | 0.59 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 4 | 0.59 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 4 | 0.59 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 4 | 0.59 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 4 | 0.59 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 4 | 0.59 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 4 | 0.59 |
| (1,572) | 1:92:A:LYS:HD2 | 1:93:A:GLU:H | 20 | 0.59 |
| (1,572) | 1:92:A:LYS:HD3 | 1:93:A:GLU:H | 20 | 0.59 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 6 | 0.59 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 6 | 0.59 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 8 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 8 | 0.59 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 8 | 0.59 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 8 | 0.59 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 8 | 0.59 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 8 | 0.59 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 20 | 0.59 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 9 | 0.59 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 16 | 0.59 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 6 | 0.59 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 6 | 0.59 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 6 | 0.59 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 15 | 0.59 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 15 | 0.59 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 15 | 0.59 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 17 | 0.58 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 17 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 17 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 17 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 17 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 17 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 17 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 17 | 0.58 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 19 | 0.58 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 19 | 0.58 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 19 | 0.58 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 19 | 0.58 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 19 | 0.58 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 19 | 0.58 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 3 | 0.58 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 3 | 0.58 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 8 | 0.58 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 8 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 2 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 2 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 2 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 2 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 2 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 2 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 3 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 3 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 3 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 3 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 3 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 3 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 8 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 8 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 8 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 8 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 8 | 0.58 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 8 | 0.58 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 5 | 0.58 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 5 | 0.58 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 5 | 0.58 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 5 | 0.58 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 5 | 0.58 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 5 | 0.58 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG2 | 6 | 0.58 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG3 | 6 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 11 | 0.58 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 11 | 0.58 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG2 | 2 | 0.58 |
| (1,3595) | 1:76:A:MET:HG2 | 1:81:A:ARG:HG3 | 2 | 0.58 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG2 | 2 | 0.58 |
| (1,3595) | 1:76:A:MET:HG3 | 1:81:A:ARG:HG3 | 2 | 0.58 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 3 | 0.58 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 3 | 0.58 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 14 | 0.58 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 14 | 0.58 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 14 | 0.58 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 14 | 0.58 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 14 | 0.58 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 14 | 0.58 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 13 | 0.58 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 7 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 9 | 0.58 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 9 | 0.58 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 9 | 0.58 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 9 | 0.58 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 9 | 0.58 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 9 | 0.58 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 16 | 0.58 |
| (1,3055) | 1:193:A:THR:HG21 | 1:195:A:ASN:HD21 | 5 | 0.58 |
| (1,3055) | 1:193:A:THR:HG22 | 1:195:A:ASN:HD21 | 5 | 0.58 |
| (1,3055) | 1:193:A:THR:HG23 | 1:195:A:ASN:HD21 | 5 | 0.58 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 13 | 0.58 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 2 | 0.58 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 10 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 8 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 8 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 9 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 9 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 11 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 11 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 14 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 14 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 16 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 16 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 20 | 0.58 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 20 | 0.58 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 13 | 0.58 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 8 | 0.58 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 11 | 0.58 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 11 | 0.58 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 11 | 0.58 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 9 | 0.58 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 9 | 0.58 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 9 | 0.58 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 12 | 0.58 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 12 | 0.58 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 1 | 0.58 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 12 | 0.58 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 12 | 0.58 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 12 | 0.58 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 13 | 0.58 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 11 | 0.58 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 8 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 8 | 0.58 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 7 | 0.58 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 9 | 0.58 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 9 | 0.58 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 9 | 0.58 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 14 | 0.58 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 7 | 0.58 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 7 | 0.58 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 7 | 0.58 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG21 | 8 | 0.58 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG22 | 8 | 0.58 |
| (1,1819) | 1:170:A:PHE:HB3 | 1:201:A:ILE:HG23 | 8 | 0.58 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 9 | 0.58 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 9 | 0.58 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 9 | 0.58 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 5 | 0.58 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 5 | 0.58 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 16 | 0.58 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 16 | 0.58 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 16 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 6 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 6 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 6 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 6 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 6 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 6 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 15 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 15 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 15 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 15 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 15 | 0.58 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 15 | 0.58 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 19 | 0.58 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 19 | 0.58 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 19 | 0.58 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 6 | 0.58 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 6 | 0.58 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 6 | 0.58 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 1 | 0.58 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 1 | 0.58 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 1 | 0.58 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 19 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 19 | 0.58 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 19 | 0.58 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 4 | 0.58 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 4 | 0.58 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 19 | 0.58 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 12 | 0.58 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 12 | 0.58 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 12 | 0.58 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 16 | 0.58 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 16 | 0.58 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 16 | 0.58 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 10 | 0.58 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 7 | 0.58 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 7 | 0.58 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 7 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 9 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 9 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 9 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 9 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 9 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 9 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 12 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 12 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 12 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 12 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 12 | 0.58 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 12 | 0.58 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB1 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB2 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB3 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB1 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB2 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB3 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB1 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB2 | 19 | 0.58 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB3 | 19 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 10 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 10 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 10 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 10 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 10 | 0.58 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 10 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 9 | 0.58 |
| (1,1002) | 1:123:A:LYS:HD3 | 1:136:A:TYR:HB3 | 11 | 0.58 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 5 | 0.58 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 7 | 0.58 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 1 | 0.58 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 17 | 0.58 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 15 | 0.58 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 15 | 0.58 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 15 | 0.58 |
| (1,782) | 1:80:A:SER:HB2 | 1:114:A:ASP:HB3 | 5 | 0.58 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 4 | 0.58 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 6 | 0.58 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 6 | 0.58 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 14 | 0.58 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 14 | 0.58 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 14 | 0.58 |
| (1,484) | 1:82:A:LEU:HG | 1:83:A:GLN:H | 1 | 0.58 |
| (1,484) | 1:82:A:LEU:HG | 1:83:A:GLN:H | 12 | 0.58 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 1 | 0.58 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 11 | 0.58 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 12 | 0.58 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 9 | 0.58 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 9 | 0.58 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 12 | 0.58 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 12 | 0.58 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 12 | 0.58 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 13 | 0.58 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 13 | 0.58 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 13 | 0.58 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 4 | 0.58 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 4 | 0.58 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 4 | 0.58 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 9 | 0.58 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 9 | 0.58 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 9 | 0.58 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 8 | 0.58 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 8 | 0.58 |
| (1,376) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 8 | 0.58 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 17 | 0.58 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 17 | 0.58 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 17 | 0.58 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 16 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 16 | 0.58 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 16 | 0.58 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 14 | 0.58 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 14 | 0.58 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 19 | 0.58 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 13 | 0.58 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 13 | 0.58 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 13 | 0.58 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 13 | 0.58 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 7 | 0.58 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 7 | 0.58 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 7 | 0.58 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 13 | 0.58 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 13 | 0.58 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 13 | 0.58 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 11 | 0.58 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 12 | 0.58 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 7 | 0.58 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 7 | 0.58 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 7 | 0.58 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 1 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 1 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 1 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 1 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 1 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 1 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 11 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 11 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 11 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 11 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 11 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 11 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 15 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 15 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 15 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 15 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 15 | 0.57 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 15 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 8 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 8 | 0.57 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 8 | 0.57 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 16 | 0.57 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 16 | 0.57 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 16 | 0.57 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 16 | 0.57 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 16 | 0.57 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 16 | 0.57 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 14 | 0.57 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 14 | 0.57 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG2 | 7 | 0.57 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG3 | 7 | 0.57 |
| (1,3615) | 1:80:A:SER:HB2 | 1:114:A:ASP:HA | 2 | 0.57 |
| (1,3615) | 1:80:A:SER:HB3 | 1:114:A:ASP:HA | 2 | 0.57 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 4 | 0.57 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 4 | 0.57 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 4 | 0.57 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 5 | 0.57 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 5 | 0.57 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 11 | 0.57 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 7 | 0.57 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 9 | 0.57 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 9 | 0.57 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 9 | 0.57 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 5 | 0.57 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 5 | 0.57 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 5 | 0.57 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 5 | 0.57 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 5 | 0.57 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 5 | 0.57 |
| (1,3090) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE21 | 4 | 0.57 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 1 | 0.57 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 20 | 0.57 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 1 | 0.57 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 1 | 0.57 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 11 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 15 | 0.57 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 19 | 0.57 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 19 | 0.57 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 19 | 0.57 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 7 | 0.57 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 15 | 0.57 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 10 | 0.57 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 10 | 0.57 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 9 | 0.57 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 12 | 0.57 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 3 | 0.57 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 18 | 0.57 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 19 | 0.57 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 19 | 0.57 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 19 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 8 | 0.57 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 8 | 0.57 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 16 | 0.57 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 16 | 0.57 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 16 | 0.57 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 6 | 0.57 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 7 | 0.57 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 9 | 0.57 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 6 | 0.57 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 3 | 0.57 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 8 | 0.57 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 6 | 0.57 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 6 | 0.57 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 6 | 0.57 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 16 | 0.57 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 16 | 0.57 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 16 | 0.57 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 19 | 0.57 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 7 | 0.57 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 7 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 7 | 0.57 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 8 | 0.57 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 8 | 0.57 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 8 | 0.57 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 10 | 0.57 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 10 | 0.57 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 10 | 0.57 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 12 | 0.57 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 12 | 0.57 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 11 | 0.57 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 11 | 0.57 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 11 | 0.57 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 15 | 0.57 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 15 | 0.57 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 15 | 0.57 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 13 | 0.57 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 13 | 0.57 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 13 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 19 | 0.57 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 19 | 0.57 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 7 | 0.57 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 12 | 0.57 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 19 | 0.57 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 19 | 0.57 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 9 | 0.57 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 3 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 2 | 0.57 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 2 | 0.57 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 2 | 0.57 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 13 | 0.57 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 13 | 0.57 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 13 | 0.57 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 12 | 0.57 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 12 | 0.57 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 12 | 0.57 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 1 | 0.57 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 17 | 0.57 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 7 | 0.57 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 3 | 0.57 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 3 | 0.57 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 3 | 0.57 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 17 | 0.57 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 17 | 0.57 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 17 | 0.57 |
| (1,956) | 1:190:A:LYS:HA | 1:190:A:LYS:HE3 | 8 | 0.57 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 12 | 0.57 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 17 | 0.57 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 17 | 0.57 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 17 | 0.57 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 1 | 0.57 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 12 | 0.57 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 10 | 0.57 |
| (1,740) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HG2 | 19 | 0.57 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 19 | 0.57 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 19 | 0.57 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 10 | 0.57 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 10 | 0.57 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 10 | 0.57 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 10 | 0.57 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 10 | 0.57 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 10 | 0.57 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 2 | 0.57 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 2 | 0.57 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 2 | 0.57 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 18 | 0.57 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 18 | 0.57 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 18 | 0.57 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 18 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 18 | 0.57 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 18 | 0.57 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 15 | 0.57 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 15 | 0.57 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 15 | 0.57 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD11 | 3 | 0.57 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD12 | 3 | 0.57 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD13 | 3 | 0.57 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD21 | 3 | 0.57 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD22 | 3 | 0.57 |
| (1,555) | 1:133:A:TRP:HE1 | 1:163:A:LEU:HD23 | 3 | 0.57 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 4 | 0.57 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 7 | 0.57 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 19 | 0.57 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 7 | 0.57 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 7 | 0.57 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 7 | 0.57 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 11 | 0.57 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 11 | 0.57 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 11 | 0.57 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 5 | 0.57 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 13 | 0.57 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 13 | 0.57 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 13 | 0.57 |
| (1,261) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HZ | 8 | 0.57 |
| (1,261) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HZ | 8 | 0.57 |
| (1,261) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HZ | 8 | 0.57 |
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 6 | 0.57 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 13 | 0.57 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 13 | 0.57 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 13 | 0.57 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 13 | 0.57 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 13 | 0.57 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 13 | 0.57 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 9 | 0.57 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 9 | 0.57 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 9 | 0.57 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 10 | 0.57 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 10 | 0.57 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 10 | 0.57 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 18 | 0.56 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 18 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 18 | 0.56 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 18 | 0.56 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 4 | 0.56 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 4 | 0.56 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 4 | 0.56 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 4 | 0.56 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 4 | 0.56 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 4 | 0.56 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 1 | 0.56 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 1 | 0.56 |
| (1,3843) | 1:137:A:ASP:H | 1:152:A:LYS:HE2 | 14 | 0.56 |
| (1,3843) | 1:137:A:ASP:H | 1:152:A:LYS:HE3 | 14 | 0.56 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 9 | 0.56 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 9 | 0.56 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 9 | 0.56 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 9 | 0.56 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 9 | 0.56 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 9 | 0.56 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 9 | 0.56 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 9 | 0.56 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 3 | 0.56 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 3 | 0.56 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 3 | 0.56 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 3 | 0.56 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 3 | 0.56 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 3 | 0.56 |
| (1,3683) | 1:94:A:ALA:H | 1:97:A:GLN:HB2 | 8 | 0.56 |
| (1,3683) | 1:94:A:ALA:H | 1:97:A:GLN:HB3 | 8 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE21 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE22 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE21 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE22 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE21 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE22 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE21 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE22 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE21 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE22 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE21 | 5 | 0.56 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE22 | 5 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 3 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 3 | 0.56 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 3 | 0.56 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 7 | 0.56 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 7 | 0.56 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 19 | 0.56 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 19 | 0.56 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 19 | 0.56 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 19 | 0.56 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 19 | 0.56 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 19 | 0.56 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 19 | 0.56 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 18 | 0.56 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 18 | 0.56 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 2 | 0.56 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 2 | 0.56 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 19 | 0.56 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 19 | 0.56 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 1 | 0.56 |
| (1,3248) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HE1 | 12 | 0.56 |
| (1,3248) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HE1 | 12 | 0.56 |
| (1,3248) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HE1 | 12 | 0.56 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 9 | 0.56 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 9 | 0.56 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 1 | 0.56 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 1 | 0.56 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB1 | 12 | 0.56 |
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB2 | 12 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3121) | 1:63:A:TYR:HE1 | 1:67:A:ALA:HB3 | 12 | 0.56 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB1 | 12 | 0.56 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB2 | 12 | 0.56 |
| (1,3121) | 1:63:A:TYR:HE2 | 1:67:A:ALA:HB3 | 12 | 0.56 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 17 | 0.56 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 17 | 0.56 |
| (1,3116) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HA | 2 | 0.56 |
| (1,3116) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HA | 2 | 0.56 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 4 | 0.56 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 4 | 0.56 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 6 | 0.56 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 6 | 0.56 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 6 | 0.56 |
| (1,3074) | 1:167:A:ASP:H | 1:196:A:ASN:HD22 | 5 | 0.56 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 1 | 0.56 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 8 | 0.56 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 6 | 0.56 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 18 | 0.56 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 18 | 0.56 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 18 | 0.56 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 16 | 0.56 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 6 | 0.56 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 6 | 0.56 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 7 | 0.56 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 7 | 0.56 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 17 | 0.56 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 15 | 0.56 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 6 | 0.56 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 6 | 0.56 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 6 | 0.56 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 10 | 0.56 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 10 | 0.56 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 10 | 0.56 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 12 | 0.56 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 6 | 0.56 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 5 | 0.56 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 13 | 0.56 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 5 | 0.56 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 5 | 0.56 |
| (1,2269) | 1:69:A:PHE:HD1 | 1:74:A:ASP:H | 8 | 0.56 |
| (1,2269) | 1:69:A:PHE:HD2 | 1:74:A:ASP:H | 8 | 0.56 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 17 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2139) | 1:48:A:ASN:H | 1:49:A:ASP:H | 11 | 0.56 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 12 | 0.56 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 11 | 0.56 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 11 | 0.56 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 11 | 0.56 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 11 | 0.56 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 11 | 0.56 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 11 | 0.56 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 19 | 0.56 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 19 | 0.56 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 19 | 0.56 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 19 | 0.56 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 19 | 0.56 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 19 | 0.56 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 8 | 0.56 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 8 | 0.56 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 8 | 0.56 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 4 | 0.56 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 4 | 0.56 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 4 | 0.56 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 13 | 0.56 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 13 | 0.56 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 13 | 0.56 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 4 | 0.56 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 4 | 0.56 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 4 | 0.56 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 1 | 0.56 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 19 | 0.56 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 19 | 0.56 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 19 | 0.56 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 6 | 0.56 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 6 | 0.56 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 6 | 0.56 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 8 | 0.56 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 8 | 0.56 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 8 | 0.56 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 9 | 0.56 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 9 | 0.56 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 9 | 0.56 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 9 | 0.56 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 19 | 0.56 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 19 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 19 | 0.56 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 19 | 0.56 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 19 | 0.56 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 19 | 0.56 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 19 | 0.56 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 3 | 0.56 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 3 | 0.56 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 3 | 0.56 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 3 | 0.56 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 3 | 0.56 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 3 | 0.56 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 16 | 0.56 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 16 | 0.56 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 16 | 0.56 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 16 | 0.56 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 16 | 0.56 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 16 | 0.56 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 16 | 0.56 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 16 | 0.56 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 16 | 0.56 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 4 | 0.56 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 4 | 0.56 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 4 | 0.56 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 13 | 0.56 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 13 | 0.56 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 6 | 0.56 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 16 | 0.56 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 17 | 0.56 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 11 | 0.56 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 20 | 0.56 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 10 | 0.56 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 3 | 0.56 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 3 | 0.56 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 3 | 0.56 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 3 | 0.56 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 5 | 0.56 |
| (1,20) | 1:47:A:THR:HG21 | 1:50:A:LEU:HA | 20 | 0.56 |
| (1,20) | 1:47:A:THR:HG22 | 1:50:A:LEU:HA | 20 | 0.56 |
| (1,20) | 1:47:A:THR:HG23 | 1:50:A:LEU:HA | 20 | 0.56 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 1 | 0.56 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 1 | 0.56 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 5 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 5 | 0.55 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 5 | 0.55 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 5 | 0.55 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 5 | 0.55 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 5 | 0.55 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 2 | 0.55 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 2 | 0.55 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 2 | 0.55 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 2 | 0.55 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 2 | 0.55 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 2 | 0.55 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 11 | 0.55 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 11 | 0.55 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 11 | 0.55 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 11 | 0.55 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 11 | 0.55 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 11 | 0.55 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 9 | 0.55 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 9 | 0.55 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 9 | 0.55 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 9 | 0.55 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 12 | 0.55 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 12 | 0.55 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 13 | 0.55 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 13 | 0.55 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 7 | 0.55 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 7 | 0.55 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 12 | 0.55 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 12 | 0.55 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 12 | 0.55 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 12 | 0.55 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 12 | 0.55 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 12 | 0.55 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 8 | 0.55 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 8 | 0.55 |
| (1,3488) | 1:54:A:ILE:HD11 | 2:11:B:CYS:H | 13 | 0.55 |
| (1,3488) | 1:54:A:ILE:HD12 | 2:11:B:CYS:H | 13 | 0.55 |
| (1,3488) | 1:54:A:ILE:HD13 | 2:11:B:CYS:H | 13 | 0.55 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 1 | 0.55 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 1 | 0.55 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 1 | 0.55 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 13 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 13 | 0.55 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 13 | 0.55 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 14 | 0.55 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 14 | 0.55 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 14 | 0.55 |
| (1,3371) | 2:10:B:TYR:HD1 | 2:21:B:MET:HG3 | 18 | 0.55 |
| (1,3371) | 2:10:B:TYR:HD2 | 2:21:B:MET:HG3 | 18 | 0.55 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 18 | 0.55 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 13 | 0.55 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 5 | 0.55 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 5 | 0.55 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 5 | 0.55 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 20 | 0.55 |
| (1,3206) | 1:88:A:GLN:HG2 | 1:90:A:HIS:HE1 | 8 | 0.55 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 3 | 0.55 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 11 | 0.55 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 11 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD1 | 1:135:A:PHE:HD1 | 1 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD1 | 1:135:A:PHE:HD2 | 1 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD2 | 1:135:A:PHE:HD1 | 1 | 0.55 |
| (1,3159) | 1:112:A:TYR:HD2 | 1:135:A:PHE:HD2 | 1 | 0.55 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 7 | 0.55 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 7 | 0.55 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 11 | 0.55 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 10 | 0.55 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 5 | 0.55 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 14 | 0.55 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 1 | 0.55 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 1 | 0.55 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 1 | 0.55 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 14 | 0.55 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 14 | 0.55 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 14 | 0.55 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 3 | 0.55 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 2 | 0.55 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 18 | 0.55 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 17 | 0.55 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 17 | 0.55 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 18 | 0.55 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 18 | 0.55 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 7 | 0.55 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 10 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG11 | 10 | 0.55 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG12 | 10 | 0.55 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG13 | 10 | 0.55 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 9 | 0.55 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 2 | 0.55 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 8 | 0.55 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 10 | 0.55 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 7 | 0.55 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 6 | 0.55 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 6 | 0.55 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 6 | 0.55 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 6 | 0.55 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 6 | 0.55 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 6 | 0.55 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 8 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 18 | 0.55 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 18 | 0.55 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 1 | 0.55 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 1 | 0.55 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 1 | 0.55 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 12 | 0.55 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 12 | 0.55 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 7 | 0.55 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 8 | 0.55 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 8 | 0.55 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG21 | 8 | 0.55 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG22 | 8 | 0.55 |
| (1,1834) | 1:222:A:ILE:HG12 | 1:223:A:THR:HG23 | 8 | 0.55 |
| (1,1731) | 1:167:A:ASP:HA | 1:196:A:ASN:HB3 | 4 | 0.55 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 5 | 0.55 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 5 | 0.55 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 5 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 15 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 15 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 17 | 0.55 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 17 | 0.55 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 1 | 0.55 |
| (1,1412) | 1:174:A:GLU:HG2 | 1:177:A:GLU:HB3 | 12 | 0.55 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 9 | 0.55 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 9 | 0.55 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 16 | 0.55 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 16 | 0.55 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 17 | 0.55 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 17 | 0.55 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 6 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 4 | 0.55 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 15 | 0.55 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 18 | 0.55 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 19 | 0.55 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 19 | 0.55 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 19 | 0.55 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 6 | 0.55 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 7 | 0.55 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 15 | 0.55 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 18 | 0.55 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 12 | 0.55 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 12 | 0.55 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 12 | 0.55 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 12 | 0.55 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 12 | 0.55 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 12 | 0.55 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 3 | 0.55 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 3 | 0.55 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 3 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 12 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 12 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 12 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 14 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 14 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 14 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 18 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 18 | 0.55 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 18 | 0.55 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 8 | 0.55 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 8 | 0.55 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 8 | 0.55 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 8 | 0.55 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 8 | 0.55 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 8 | 0.55 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 15 | 0.55 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 15 | 0.55 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 15 | 0.55 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 4 | 0.55 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 4 | 0.55 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 3 | 0.55 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 3 | 0.55 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 3 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 4 | 0.55 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 4 | 0.55 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 4 | 0.55 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 17 | 0.55 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 17 | 0.55 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 17 | 0.55 |
| (1,386) | 1:75:A:ILE:HD11 | 1:84:A:ALA:H | 4 | 0.55 |
| (1,386) | 1:75:A:ILE:HD12 | 1:84:A:ALA:H | 4 | 0.55 |
| (1,386) | 1:75:A:ILE:HD13 | 1:84:A:ALA:H | 4 | 0.55 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 3 | 0.55 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 3 | 0.55 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 3 | 0.55 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 17 | 0.55 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 17 | 0.55 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 17 | 0.55 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 10 | 0.55 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 10 | 0.55 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 2 | 0.55 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 2 | 0.55 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 2 | 0.55 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 3 | 0.55 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 3 | 0.55 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 3 | 0.55 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 3 | 0.55 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 4 | 0.55 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 4 | 0.55 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 4 | 0.55 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 4 | 0.55 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 4 | 0.55 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 4 | 0.55 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 19 | 0.55 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 19 | 0.55 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 19 | 0.55 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 20 | 0.54 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 20 | 0.54 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 20 | 0.54 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 20 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 4 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 4 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 16 | 0.54 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 16 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 12 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 12 | 0.54 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 12 | 0.54 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 13 | 0.54 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 13 | 0.54 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 13 | 0.54 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 13 | 0.54 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 13 | 0.54 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 13 | 0.54 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 13 | 0.54 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 13 | 0.54 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 5 | 0.54 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 5 | 0.54 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 5 | 0.54 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 5 | 0.54 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 5 | 0.54 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 10 | 0.54 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG21 | 13 | 0.54 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG22 | 13 | 0.54 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG23 | 13 | 0.54 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 18 | 0.54 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 18 | 0.54 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 18 | 0.54 |
| (1,3281) | 1:54:A:ILE:HD11 | 1:69:A:PHE:HZ | 12 | 0.54 |
| (1,3281) | 1:54:A:ILE:HD12 | 1:69:A:PHE:HZ | 12 | 0.54 |
| (1,3281) | 1:54:A:ILE:HD13 | 1:69:A:PHE:HZ | 12 | 0.54 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 16 | 0.54 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 3 | 0.54 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 15 | 0.54 |
| (1,3159) | 1:112:A:TYR:HD1 | 1:135:A:PHE:HD1 | 17 | 0.54 |
| (1,3159) | 1:112:A:TYR:HD1 | 1:135:A:PHE:HD2 | 17 | 0.54 |
| (1,3159) | 1:112:A:TYR:HD2 | 1:135:A:PHE:HD1 | 17 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3159) | 1:112:A:TYR:HD2 | 1:135:A:PHE:HD2 | 17 | 0.54 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 3 | 0.54 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 3 | 0.54 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 5 | 0.54 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 6 | 0.54 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 9 | 0.54 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 9 | 0.54 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 9 | 0.54 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 4 | 0.54 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 4 | 0.54 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 9 | 0.54 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 11 | 0.54 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 2 | 0.54 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 13 | 0.54 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 18 | 0.54 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 18 | 0.54 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 18 | 0.54 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 9 | 0.54 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 20 | 0.54 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 20 | 0.54 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 20 | 0.54 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 14 | 0.54 |
| (1,2563) | 1:137:A:ASP:H | 1:152:A:LYS:HB2 | 10 | 0.54 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 16 | 0.54 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 17 | 0.54 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 3 | 0.54 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 19 | 0.54 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 19 | 0.54 |
| (1,2141) | 1:49:A:ASP:HA | 1:50:A:LEU:H | 16 | 0.54 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 19 | 0.54 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 19 | 0.54 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 16 | 0.54 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 20 | 0.54 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 20 | 0.54 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 20 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD2 | 17 | 0.54 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD3 | 17 | 0.54 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD2 | 17 | 0.54 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD3 | 17 | 0.54 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD2 | 17 | 0.54 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD3 | 17 | 0.54 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 5 | 0.54 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 8 | 0.54 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 8 | 0.54 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 8 | 0.54 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 16 | 0.54 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 19 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 7 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 7 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 7 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 17 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 17 | 0.54 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 17 | 0.54 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 11 | 0.54 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 11 | 0.54 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 4 | 0.54 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 4 | 0.54 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 4 | 0.54 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 4 | 0.54 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 4 | 0.54 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 4 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 8 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 8 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 8 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 15 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 15 | 0.54 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 15 | 0.54 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 14 | 0.54 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 14 | 0.54 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 14 | 0.54 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 7 | 0.54 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 7 | 0.54 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 7 | 0.54 |
| (1,1413) | 1:174:A:GLU:HG3 | 1:177:A:GLU:HB3 | 12 | 0.54 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 17 | 0.54 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 3 | 0.54 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 3 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 19 | 0.54 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 11 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 2 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 2 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 2 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 11 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 11 | 0.54 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 11 | 0.54 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 20 | 0.54 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 16 | 0.54 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 5 | 0.54 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 12 | 0.54 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 1 | 0.54 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 1 | 0.54 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 11 | 0.54 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 11 | 0.54 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 11 | 0.54 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 11 | 0.54 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 11 | 0.54 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 11 | 0.54 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 13 | 0.54 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 13 | 0.54 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 13 | 0.54 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 6 | 0.54 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 19 | 0.54 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 2 | 0.54 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 17 | 0.54 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 18 | 0.54 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 2 | 0.54 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 2 | 0.54 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 2 | 0.54 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 18 | 0.54 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 20 | 0.54 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 20 | 0.54 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 20 | 0.54 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 20 | 0.54 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 20 | 0.54 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 20 | 0.54 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 20 | 0.54 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 9 | 0.54 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 9 | 0.54 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 9 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 17 | 0.54 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 17 | 0.54 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 17 | 0.54 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 3 | 0.54 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 3 | 0.54 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 3 | 0.54 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 1 | 0.54 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 8 | 0.54 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 8 | 0.54 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 8 | 0.54 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 18 | 0.54 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 18 | 0.54 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 18 | 0.54 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 17 | 0.54 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 10 | 0.54 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 10 | 0.54 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 10 | 0.54 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 19 | 0.54 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 1 | 0.54 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 1 | 0.54 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 1 | 0.54 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 16 | 0.54 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 14 | 0.54 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 13 | 0.53 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 13 | 0.53 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 13 | 0.53 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 13 | 0.53 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 13 | 0.53 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 13 | 0.53 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 14 | 0.53 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 14 | 0.53 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 14 | 0.53 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 14 | 0.53 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 14 | 0.53 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 14 | 0.53 |
| (1,3768) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG13 | 5 | 0.53 |
| (1,3768) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 5 | 0.53 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 6 | 0.53 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 6 | 0.53 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 11 | 0.53 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 11 | 0.53 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 17 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 17 | 0.53 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 17 | 0.53 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 17 | 0.53 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 17 | 0.53 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 17 | 0.53 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 4 | 0.53 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 4 | 0.53 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 4 | 0.53 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 2 | 0.53 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 2 | 0.53 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 2 | 0.53 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 8 | 0.53 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 8 | 0.53 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 19 | 0.53 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 19 | 0.53 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 19 | 0.53 |
| (1,3067) | 1:167:A:ASP:HA | 1:196:A:ASN:HD21 | 19 | 0.53 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 10 | 0.53 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 8 | 0.53 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 8 | 0.53 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 8 | 0.53 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 6 | 0.53 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 2 | 0.53 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 2 | 0.53 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 3 | 0.53 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 9 | 0.53 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 10 | 0.53 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 10 | 0.53 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 10 | 0.53 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 13 | 0.53 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 13 | 0.53 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 13 | 0.53 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 12 | 0.53 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 13 | 0.53 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 13 | 0.53 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 6 | 0.53 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 8 | 0.53 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 17 | 0.53 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 12 | 0.53 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 13 | 0.53 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 13 | 0.53 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 13 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 5 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 5 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 5 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 11 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 11 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 11 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 18 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 18 | 0.53 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 18 | 0.53 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 15 | 0.53 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 15 | 0.53 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 15 | 0.53 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 5 | 0.53 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 8 | 0.53 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 18 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 7 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 7 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 7 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 8 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 8 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 8 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD11 | 13 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD12 | 13 | 0.53 |
| (1,1690) | 1:192:A:ILE:H | 1:194:A:ILE:HD13 | 13 | 0.53 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 16 | 0.53 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 16 | 0.53 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 16 | 0.53 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 3 | 0.53 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 3 | 0.53 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 3 | 0.53 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 8 | 0.53 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 18 | 0.53 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 18 | 0.53 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 18 | 0.53 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 6 | 0.53 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 20 | 0.53 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 7 | 0.53 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 7 | 0.53 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 15 | 0.53 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 15 | 0.53 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 4 | 0.53 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 8 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 8 | 0.53 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 8 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 4 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 4 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 4 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 17 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 17 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 17 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 18 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 18 | 0.53 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 18 | 0.53 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 8 | 0.53 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 8 | 0.53 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 8 | 0.53 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 4 | 0.53 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 20 | 0.53 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 6 | 0.53 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 16 | 0.53 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 11 | 0.53 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 11 | 0.53 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 11 | 0.53 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 15 | 0.53 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 15 | 0.53 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 15 | 0.53 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 19 | 0.53 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 19 | 0.53 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 19 | 0.53 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 13 | 0.53 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 13 | 0.53 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 13 | 0.53 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 12 | 0.53 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 19 | 0.53 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 2 | 0.53 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 2 | 0.53 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 2 | 0.53 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 2 | 0.53 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 2 | 0.53 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 2 | 0.53 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 19 | 0.53 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 19 | 0.53 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 19 | 0.53 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 19 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 19 | 0.53 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 19 | 0.53 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 14 | 0.53 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 14 | 0.53 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 14 | 0.53 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 14 | 0.53 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 14 | 0.53 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 14 | 0.53 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 8 | 0.53 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 8 | 0.53 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 8 | 0.53 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 13 | 0.53 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 13 | 0.53 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 13 | 0.53 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 9 | 0.53 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 9 | 0.53 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 9 | 0.53 |
| (1,613) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG2 | 15 | 0.53 |
| (1,613) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG2 | 15 | 0.53 |
| (1,613) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG2 | 15 | 0.53 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 19 | 0.53 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 19 | 0.53 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 19 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 1 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 1 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 1 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 7 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 7 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 7 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 14 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 14 | 0.53 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 14 | 0.53 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 14 | 0.53 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 15 | 0.53 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 15 | 0.53 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 15 | 0.53 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 4 | 0.53 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 8 | 0.53 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 8 | 0.53 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 8 | 0.53 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 5 | 0.53 |
| (1,348) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HB2 | 1 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,348) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HB2 | 1 | 0.53 |
| (1,348) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HB2 | 1 | 0.53 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 7 | 0.53 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 7 | 0.53 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 7 | 0.53 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 13 | 0.53 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 13 | 0.53 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 13 | 0.53 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 10 | 0.53 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 10 | 0.53 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 10 | 0.53 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 11 | 0.53 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 12 | 0.53 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 12 | 0.53 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 12 | 0.53 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 19 | 0.53 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 14 | 0.53 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 4 | 0.53 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 19 | 0.53 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 16 | 0.53 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 16 | 0.53 |
| (1,3990) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 17 | 0.52 |
| (1,3990) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 17 | 0.52 |
| (1,3990) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 17 | 0.52 |
| (1,3990) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 17 | 0.52 |
| (1,3990) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 17 | 0.52 |
| (1,3990) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 17 | 0.52 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 8 | 0.52 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 8 | 0.52 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 8 | 0.52 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 8 | 0.52 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 8 | 0.52 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 8 | 0.52 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE2 | 9 | 0.52 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE3 | 9 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 14 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 14 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 14 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 14 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 14 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 14 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 16 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 16 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 16 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 16 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 16 | 0.52 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 16 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 14 | 0.52 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 14 | 0.52 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 8 | 0.52 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 8 | 0.52 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 13 | 0.52 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 13 | 0.52 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 13 | 0.52 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 13 | 0.52 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 13 | 0.52 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 13 | 0.52 |
| (1,3505) | 1:51:A:PRO:HB3 | 2:7:B:PRO:HD3 | 8 | 0.52 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 2 | 0.52 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 2 | 0.52 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 2 | 0.52 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 8 | 0.52 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 8 | 0.52 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 8 | 0.52 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 8 | 0.52 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 8 | 0.52 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 8 | 0.52 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 1 | 0.52 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 1 | 0.52 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 1 | 0.52 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 17 | 0.52 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 13 | 0.52 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 13 | 0.52 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 1 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 13 | 0.52 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 4 | 0.52 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 16 | 0.52 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 16 | 0.52 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 16 | 0.52 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 7 | 0.52 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 13 | 0.52 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 19 | 0.52 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 19 | 0.52 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 10 | 0.52 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 20 | 0.52 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 5 | 0.52 |
| (1,2866) | 1:185:A:LYS:H | 1:216:A:LEU:HG | 12 | 0.52 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 8 | 0.52 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 8 | 0.52 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 8 | 0.52 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 5 | 0.52 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 8 | 0.52 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 14 | 0.52 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 2 | 0.52 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 10 | 0.52 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 12 | 0.52 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 12 | 0.52 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 19 | 0.52 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 4 | 0.52 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 4 | 0.52 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 4 | 0.52 |
| (1,2358) | 1:69:A:PHE:HE1 | 1:89:A:LEU:H | 8 | 0.52 |
| (1,2358) | 1:69:A:PHE:HE2 | 1:89:A:LEU:H | 8 | 0.52 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 13 | 0.52 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 17 | 0.52 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 19 | 0.52 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 20 | 0.52 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 6 | 0.52 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 2 | 0.52 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 2 | 0.52 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 2 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 9 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 9 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 15 | 0.52 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 15 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 2 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 2 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 2 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 6 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 6 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 6 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 7 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 7 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 7 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 10 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 10 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 10 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 14 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 14 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 14 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 20 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 20 | 0.52 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 20 | 0.52 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 18 | 0.52 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 16 | 0.52 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 6 | 0.52 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 19 | 0.52 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 14 | 0.52 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 14 | 0.52 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 14 | 0.52 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 19 | 0.52 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 19 | 0.52 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 19 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 13 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 13 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 13 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 13 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 13 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 13 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 18 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 18 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 18 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 18 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 18 | 0.52 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 18 | 0.52 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 1 | 0.52 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 1 | 0.52 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 1 | 0.52 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 4 | 0.52 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 4 | 0.52 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 4 | 0.52 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 10 | 0.52 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 10 | 0.52 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 10 | 0.52 |
| (1,1441) | 1:142:A:THR:HG21 | 1:178:A:ALA:HA | 12 | 0.52 |
| (1,1441) | 1:142:A:THR:HG22 | 1:178:A:ALA:HA | 12 | 0.52 |
| (1,1441) | 1:142:A:THR:HG23 | 1:178:A:ALA:HA | 12 | 0.52 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 11 | 0.52 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 11 | 0.52 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 12 | 0.52 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 12 | 0.52 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 7 | 0.52 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 14 | 0.52 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 1 | 0.52 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 1 | 0.52 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 1 | 0.52 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 1 | 0.52 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 1 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 1 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 1 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 1 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 5 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 5 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 5 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 10 | 0.52 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 10 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 10 | 0.52 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 1 | 0.52 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 9 | 0.52 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 9 | 0.52 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 9 | 0.52 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 9 | 0.52 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 9 | 0.52 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 9 | 0.52 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 17 | 0.52 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 17 | 0.52 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 17 | 0.52 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 17 | 0.52 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 17 | 0.52 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 17 | 0.52 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 20 | 0.52 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 20 | 0.52 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 20 | 0.52 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG11 | 2 | 0.52 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG12 | 2 | 0.52 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG13 | 2 | 0.52 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 12 | 0.52 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 12 | 0.52 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 12 | 0.52 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 3 | 0.52 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 3 | 0.52 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 3 | 0.52 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 14 | 0.52 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 14 | 0.52 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 14 | 0.52 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 4 | 0.52 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 4 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 11 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 11 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 11 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 11 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 11 | 0.52 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 11 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 1 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 1 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 1 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 2 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 2 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 2 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 3 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 3 | 0.52 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 3 | 0.52 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 5 | 0.52 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 13 | 0.52 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 13 | 0.52 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 13 | 0.52 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 16 | 0.52 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 16 | 0.52 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 16 | 0.52 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 3 | 0.52 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 9 | 0.52 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 5 | 0.52 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 5 | 0.52 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 15 | 0.52 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 11 | 0.52 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 11 | 0.52 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 11 | 0.52 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 8 | 0.52 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 8 | 0.52 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 8 | 0.52 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 15 | 0.52 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 15 | 0.52 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 15 | 0.52 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 5 | 0.52 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 5 | 0.52 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 5 | 0.52 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 11 | 0.52 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 11 | 0.52 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 11 | 0.52 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 17 | 0.52 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 17 | 0.52 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 17 | 0.52 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 4 | 0.52 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 4 | 0.52 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 4 | 0.52 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 15 | 0.52 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 15 | 0.52 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 15 | 0.52 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 7 | 0.52 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 7 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 8 | 0.52 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 8 | 0.52 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 8 | 0.52 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 8 | 0.52 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 3 | 0.52 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 10 | 0.52 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 18 | 0.52 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 2 | 0.52 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 2 | 0.52 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 2 | 0.52 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 11 | 0.52 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 11 | 0.52 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 11 | 0.52 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 9 | 0.52 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 9 | 0.52 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 9 | 0.52 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 8 | 0.52 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 9 | 0.52 |
| (1,26) | 1:158:A:ASP:HB3 | 1:161:A:LYS:HG2 | 1 | 0.52 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 17 | 0.51 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 17 | 0.51 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 20 | 0.51 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 20 | 0.51 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 20 | 0.51 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 20 | 0.51 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 20 | 0.51 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 20 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 1 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 1 | 0.51 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 1 | 0.51 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 15 | 0.51 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 15 | 0.51 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 15 | 0.51 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 15 | 0.51 |
| (1,3605) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HA | 20 | 0.51 |
| (1,3605) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HA | 20 | 0.51 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 1 | 0.51 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 1 | 0.51 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 2 | 0.51 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 2 | 0.51 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 2 | 0.51 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 2 | 0.51 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 1 | 0.51 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 1 | 0.51 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 1 | 0.51 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 1 | 0.51 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 1 | 0.51 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 1 | 0.51 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 10 | 0.51 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 10 | 0.51 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 10 | 0.51 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 9 | 0.51 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 13 | 0.51 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 13 | 0.51 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 13 | 0.51 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 20 | 0.51 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 20 | 0.51 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 20 | 0.51 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 5 | 0.51 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 5 | 0.51 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 5 | 0.51 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 3 | 0.51 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 3 | 0.51 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 1 | 0.51 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 2 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 5 | 0.51 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 5 | 0.51 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 20 | 0.51 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 20 | 0.51 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 18 | 0.51 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 18 | 0.51 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 18 | 0.51 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 5 | 0.51 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 12 | 0.51 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 17 | 0.51 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 13 | 0.51 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 13 | 0.51 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 19 | 0.51 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 14 | 0.51 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 10 | 0.51 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 10 | 0.51 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 10 | 0.51 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 6 | 0.51 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 10 | 0.51 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 4 | 0.51 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 7 | 0.51 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 20 | 0.51 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 18 | 0.51 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 12 | 0.51 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 12 | 0.51 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 12 | 0.51 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 7 | 0.51 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 11 | 0.51 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 11 | 0.51 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 12 | 0.51 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 12 | 0.51 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 3 | 0.51 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 15 | 0.51 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 5 | 0.51 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 4 | 0.51 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 1 | 0.51 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 1 | 0.51 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 1 | 0.51 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 12 | 0.51 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 12 | 0.51 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 12 | 0.51 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 17 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 5 | 0.51 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 5 | 0.51 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 5 | 0.51 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 5 | 0.51 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 5 | 0.51 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 5 | 0.51 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 4 | 0.51 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 4 | 0.51 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 4 | 0.51 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 17 | 0.51 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 17 | 0.51 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 17 | 0.51 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 18 | 0.51 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 13 | 0.51 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 13 | 0.51 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 13 | 0.51 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 3 | 0.51 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 3 | 0.51 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 3 | 0.51 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 17 | 0.51 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 17 | 0.51 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 17 | 0.51 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 19 | 0.51 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 19 | 0.51 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 19 | 0.51 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 5 | 0.51 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 5 | 0.51 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 5 | 0.51 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 16 | 0.51 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 16 | 0.51 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 16 | 0.51 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 14 | 0.51 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 14 | 0.51 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 14 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 9 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 9 | 0.51 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 9 | 0.51 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 11 | 0.51 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 16 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 5 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 5 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 5 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 7 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 7 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 7 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 13 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 13 | 0.51 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 13 | 0.51 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 14 | 0.51 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 2 | 0.51 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 15 | 0.51 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 11 | 0.51 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 6 | 0.51 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 6 | 0.51 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 6 | 0.51 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 13 | 0.51 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 1 | 0.51 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 4 | 0.51 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 10 | 0.51 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 8 | 0.51 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 8 | 0.51 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 8 | 0.51 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 12 | 0.51 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 12 | 0.51 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 12 | 0.51 |
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 18 | 0.51 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 18 | 0.51 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 18 | 0.51 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 9 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 4 | 0.51 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 4 | 0.51 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 4 | 0.51 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 20 | 0.51 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 20 | 0.51 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 20 | 0.51 |
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 6 | 0.51 |
| (1,628) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD2 | 8 | 0.51 |
| (1,628) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD2 | 8 | 0.51 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 10 | 0.51 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 10 | 0.51 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 10 | 0.51 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 8 | 0.51 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 8 | 0.51 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 12 | 0.51 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 12 | 0.51 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 8 | 0.51 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 13 | 0.51 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 2 | 0.51 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 2 | 0.51 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 2 | 0.51 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 2 | 0.51 |
| (1,183) | 1:58:A:HIS:HB3 | 2:12:B:ASN:HD22 | 20 | 0.51 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 3 | 0.5 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 3 | 0.5 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 2 | 0.5 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 2 | 0.5 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 2 | 0.5 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 2 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 2 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 2 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 2 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 2 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 2 | 0.5 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 2 | 0.5 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 10 | 0.5 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 10 | 0.5 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 14 | 0.5 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 14 | 0.5 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 15 | 0.5 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 15 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 20 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 20 | 0.5 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 20 | 0.5 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 9 | 0.5 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 9 | 0.5 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 9 | 0.5 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 9 | 0.5 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 9 | 0.5 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 9 | 0.5 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 18 | 0.5 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 18 | 0.5 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 18 | 0.5 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 18 | 0.5 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 19 | 0.5 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 19 | 0.5 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 5 | 0.5 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 8 | 0.5 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 11 | 0.5 |
| (1,3508) | 1:51:A:PRO:HB2 | 2:7:B:PRO:HD2 | 12 | 0.5 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 2 | 0.5 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 2 | 0.5 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 2 | 0.5 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 2 | 0.5 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 2 | 0.5 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 2 | 0.5 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 5 | 0.5 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 5 | 0.5 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 5 | 0.5 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 20 | 0.5 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 20 | 0.5 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 20 | 0.5 |
| (1,3488) | 1:54:A:ILE:HD11 | 2:11:B:CYS:H | 2 | 0.5 |
| (1,3488) | 1:54:A:ILE:HD12 | 2:11:B:CYS:H | 2 | 0.5 |
| (1,3488) | 1:54:A:ILE:HD13 | 2:11:B:CYS:H | 2 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD2 | 19 | 0.5 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD3 | 19 | 0.5 |
| (1,3277) | 1:69:A:PHE:HD1 | 1:87:A:VAL:HB | 12 | 0.5 |
| (1,3277) | 1:69:A:PHE:HD2 | 1:87:A:VAL:HB | 12 | 0.5 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 6 | 0.5 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 6 | 0.5 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 12 | 0.5 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 13 | 0.5 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 13 | 0.5 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 13 | 0.5 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 8 | 0.5 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 8 | 0.5 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 20 | 0.5 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 20 | 0.5 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE1 | 4 | 0.5 |
| (1,3128) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HE2 | 4 | 0.5 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 18 | 0.5 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 19 | 0.5 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 11 | 0.5 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 3 | 0.5 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 3 | 0.5 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 6 | 0.5 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 13 | 0.5 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 13 | 0.5 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 13 | 0.5 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 13 | 0.5 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 5 | 0.5 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 11 | 0.5 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 3 | 0.5 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 3 | 0.5 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 3 | 0.5 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 20 | 0.5 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 20 | 0.5 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 20 | 0.5 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 5 | 0.5 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 6 | 0.5 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 6 | 0.5 |
| (1,2190) | 1:58:A:HIS:H | 2:12:B:ASN:HD22 | 5 | 0.5 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 2 | 0.5 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 2 | 0.5 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 2 | 0.5 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 17 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 17 | 0.5 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 17 | 0.5 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 11 | 0.5 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 11 | 0.5 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 11 | 0.5 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 13 | 0.5 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 1 | 0.5 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 1 | 0.5 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 1 | 0.5 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 19 | 0.5 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 12 | 0.5 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 12 | 0.5 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 7 | 0.5 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 2 | 0.5 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 2 | 0.5 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 2 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 11 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 11 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 11 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 20 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 20 | 0.5 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 20 | 0.5 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 4 | 0.5 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE2 | 11 | 0.5 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE3 | 11 | 0.5 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE2 | 11 | 0.5 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE3 | 11 | 0.5 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 10 | 0.5 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG21 | 19 | 0.5 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG22 | 19 | 0.5 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG23 | 19 | 0.5 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 15 | 0.5 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 15 | 0.5 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 15 | 0.5 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 18 | 0.5 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 18 | 0.5 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 18 | 0.5 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 2 | 0.5 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 3 | 0.5 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 14 | 0.5 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 6 | 0.5 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 13 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 18 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 2 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 2 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 2 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 2 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 2 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 2 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 6 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 6 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 6 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 6 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 6 | 0.5 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 6 | 0.5 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 4 | 0.5 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 12 | 0.5 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 12 | 0.5 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 12 | 0.5 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 1 | 0.5 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 1 | 0.5 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 1 | 0.5 |
| (1,1050) | 1:139:A:SER:HB3 | 1:150:A:SER:HA | 12 | 0.5 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 5 | 0.5 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 5 | 0.5 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 18 | 0.5 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 11 | 0.5 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 14 | 0.5 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 14 | 0.5 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 15 | 0.5 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 14 | 0.5 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 11 | 0.5 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 11 | 0.5 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 11 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 15 | 0.5 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 15 | 0.5 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 15 | 0.5 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 9 | 0.5 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 3 | 0.5 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 3 | 0.5 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 3 | 0.5 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 3 | 0.5 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 3 | 0.5 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 3 | 0.5 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 6 | 0.5 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 6 | 0.5 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 6 | 0.5 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD21 | 12 | 0.5 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD22 | 12 | 0.5 |
| (1,559) | 1:185:A:LYS:H | 1:216:A:LEU:HD23 | 12 | 0.5 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 17 | 0.5 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 10 | 0.5 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 11 | 0.5 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 14 | 0.5 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 14 | 0.5 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 14 | 0.5 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 14 | 0.5 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 14 | 0.5 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 14 | 0.5 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 18 | 0.5 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 18 | 0.5 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 18 | 0.5 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 10 | 0.5 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 10 | 0.5 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 9 | 0.5 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 14 | 0.5 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 1 | 0.5 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 19 | 0.5 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 7 | 0.5 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 7 | 0.5 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 7 | 0.5 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 6 | 0.5 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 6 | 0.5 |
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 6 | 0.5 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 6 | 0.5 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 6 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 6 | 0.5 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 14 | 0.5 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 14 | 0.5 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 14 | 0.5 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 8 | 0.5 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 8 | 0.5 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 8 | 0.5 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 8 | 0.5 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 8 | 0.5 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 8 | 0.5 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 10 | 0.5 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 10 | 0.5 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 10 | 0.5 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 4 | 0.5 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 3 | 0.5 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 1 | 0.5 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 13 | 0.5 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 13 | 0.5 |
| (1,4019) | 2:12:B:ASN:HD22 | 2:13:B:ARG:HB2 | 10 | 0.49 |
| (1,4019) | 2:12:B:ASN:HD22 | 2:13:B:ARG:HB3 | 10 | 0.49 |
| (1,3990) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 12 | 0.49 |
| (1,3990) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 12 | 0.49 |
| (1,3990) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 12 | 0.49 |
| (1,3990) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 12 | 0.49 |
| (1,3990) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 12 | 0.49 |
| (1,3990) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 12 | 0.49 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 2 | 0.49 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 2 | 0.49 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 2 | 0.49 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 2 | 0.49 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 2 | 0.49 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 2 | 0.49 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 12 | 0.49 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 12 | 0.49 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 12 | 0.49 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 12 | 0.49 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 12 | 0.49 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 12 | 0.49 |
| (1,3834) | 1:127:A:ASN:HB2 | 1:131:A:LYS:H | 5 | 0.49 |
| (1,3834) | 1:127:A:ASN:HB3 | 1:131:A:LYS:H | 5 | 0.49 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD11 | 5 | 0.49 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD12 | 5 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD13 | 5 | 0.49 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 5 | 0.49 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 5 | 0.49 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 5 | 0.49 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 20 | 0.49 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 20 | 0.49 |
| (1,3605) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HA | 18 | 0.49 |
| (1,3605) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HA | 18 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 7 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 7 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 7 | 0.49 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 7 | 0.49 |
| (1,3530) | 1:63:A:TYR:HE1 | 2:21:B:MET:HB2 | 4 | 0.49 |
| (1,3530) | 1:63:A:TYR:HE2 | 2:21:B:MET:HB2 | 4 | 0.49 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 13 | 0.49 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 13 | 0.49 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 13 | 0.49 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 5 | 0.49 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 5 | 0.49 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 5 | 0.49 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 9 | 0.49 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 9 | 0.49 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 9 | 0.49 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 10 | 0.49 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 10 | 0.49 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 10 | 0.49 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 19 | 0.49 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 19 | 0.49 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 19 | 0.49 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 16 | 0.49 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 12 | 0.49 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 15 | 0.49 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 17 | 0.49 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 2 | 0.49 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 2 | 0.49 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 5 | 0.49 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 5 | 0.49 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 7 | 0.49 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 7 | 0.49 |
| (1,3116) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HA | 7 | 0.49 |
| (1,3116) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HA | 7 | 0.49 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 20 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 2 | 0.49 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 6 | 0.49 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 7 | 0.49 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 1 | 0.49 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 7 | 0.49 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 14 | 0.49 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 20 | 0.49 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 20 | 0.49 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 20 | 0.49 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 11 | 0.49 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 15 | 0.49 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 1 | 0.49 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 19 | 0.49 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 1 | 0.49 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 7 | 0.49 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 18 | 0.49 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 18 | 0.49 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 18 | 0.49 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 5 | 0.49 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 5 | 0.49 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 5 | 0.49 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 18 | 0.49 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 19 | 0.49 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 3 | 0.49 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 1 | 0.49 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 7 | 0.49 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 7 | 0.49 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 7 | 0.49 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 16 | 0.49 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 16 | 0.49 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 16 | 0.49 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 3 | 0.49 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 3 | 0.49 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 3 | 0.49 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 7 | 0.49 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 4 | 0.49 |
| (1,1727) | 1:168:A:ALA:H | 1:196:A:ASN:HB3 | 4 | 0.49 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 15 | 0.49 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 15 | 0.49 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 15 | 0.49 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 9 | 0.49 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 9 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 9 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 8 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 8 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 8 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 10 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 10 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 10 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 13 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 13 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 13 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 17 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 17 | 0.49 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 17 | 0.49 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 10 | 0.49 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 18 | 0.49 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 18 | 0.49 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 8 | 0.49 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 7 | 0.49 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 19 | 0.49 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 19 | 0.49 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 19 | 0.49 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 20 | 0.49 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 20 | 0.49 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 20 | 0.49 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 4 | 0.49 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 16 | 0.49 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 4 | 0.49 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 4 | 0.49 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 5 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 2 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 2 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 2 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 14 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 14 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 14 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 16 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 16 | 0.49 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 16 | 0.49 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 2 | 0.49 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 12 | 0.49 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 15 | 0.49 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 16 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 16 | 0.49 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 16 | 0.49 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 16 | 0.49 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 16 | 0.49 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 16 | 0.49 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 1 | 0.49 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 2 | 0.49 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 2 | 0.49 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 2 | 0.49 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 13 | 0.49 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 13 | 0.49 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 13 | 0.49 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 13 | 0.49 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 13 | 0.49 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 13 | 0.49 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 15 | 0.49 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 15 | 0.49 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 17 | 0.49 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 17 | 0.49 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 17 | 0.49 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 14 | 0.49 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 17 | 0.49 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 8 | 0.49 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 15 | 0.49 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 15 | 0.49 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 18 | 0.49 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 18 | 0.49 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 18 | 0.49 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 20 | 0.49 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 20 | 0.49 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 20 | 0.49 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 19 | 0.49 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 19 | 0.49 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 19 | 0.49 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 2 | 0.49 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 2 | 0.49 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 2 | 0.49 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 10 | 0.49 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 10 | 0.49 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 10 | 0.49 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 15 | 0.49 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 15 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 15 | 0.49 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 15 | 0.49 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 15 | 0.49 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 15 | 0.49 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG2 | 15 | 0.49 |
| (1,116) | 1:54:A:ILE:HD11 | 1:76:A:MET:HG3 | 15 | 0.49 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG2 | 15 | 0.49 |
| (1,116) | 1:54:A:ILE:HD12 | 1:76:A:MET:HG3 | 15 | 0.49 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG2 | 15 | 0.49 |
| (1,116) | 1:54:A:ILE:HD13 | 1:76:A:MET:HG3 | 15 | 0.49 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 10 | 0.49 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 20 | 0.48 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 20 | 0.48 |
| (1,3949) | 1:193:A:THR:HB | 1:195:A:ASN:HD21 | 5 | 0.48 |
| (1,3949) | 1:193:A:THR:HB | 1:195:A:ASN:HD22 | 5 | 0.48 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 14 | 0.48 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 14 | 0.48 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 9 | 0.48 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 9 | 0.48 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB2 | 9 | 0.48 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB3 | 9 | 0.48 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB2 | 9 | 0.48 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB3 | 9 | 0.48 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB2 | 9 | 0.48 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB3 | 9 | 0.48 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 6 | 0.48 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 6 | 0.48 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 6 | 0.48 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 20 | 0.48 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 20 | 0.48 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 20 | 0.48 |
| (1,3505) | 1:51:A:PRO:HB3 | 2:7:B:PRO:HD3 | 12 | 0.48 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 1 | 0.48 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 1 | 0.48 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 1 | 0.48 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 1 | 0.48 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 1 | 0.48 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 1 | 0.48 |
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 10 | 0.48 |
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 10 | 0.48 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 10 | 0.48 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 1 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 1 | 0.48 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 3 | 0.48 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 18 | 0.48 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 13 | 0.48 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 10 | 0.48 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 10 | 0.48 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 18 | 0.48 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 18 | 0.48 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 14 | 0.48 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 11 | 0.48 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 11 | 0.48 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 11 | 0.48 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 13 | 0.48 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 13 | 0.48 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 7 | 0.48 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 7 | 0.48 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 7 | 0.48 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 15 | 0.48 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 9 | 0.48 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 14 | 0.48 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 3 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 6 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 6 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 6 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 8 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 8 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 8 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 17 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 17 | 0.48 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 17 | 0.48 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 6 | 0.48 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 11 | 0.48 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 7 | 0.48 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 1 | 0.48 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 1 | 0.48 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 14 | 0.48 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 14 | 0.48 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 9 | 0.48 |
| (1,2341) | 1:125:A:TRP:HE3 | 1:135:A:PHE:H | 10 | 0.48 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 16 | 0.48 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 2 | 0.48 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 7 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 7 | 0.48 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 7 | 0.48 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 7 | 0.48 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 10 | 0.48 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 10 | 0.48 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 10 | 0.48 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 13 | 0.48 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 13 | 0.48 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 13 | 0.48 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 4 | 0.48 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 4 | 0.48 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 4 | 0.48 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB2 | 15 | 0.48 |
| (1,1957) | 1:212:A:LYS:HA | 1:215:A:GLU:HB3 | 15 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 1 | 0.48 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 1 | 0.48 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 12 | 0.48 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 12 | 0.48 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 12 | 0.48 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 1 | 0.48 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 15 | 0.48 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 15 | 0.48 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 19 | 0.48 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 16 | 0.48 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 10 | 0.48 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 4 | 0.48 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 4 | 0.48 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 4 | 0.48 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 1 | 0.48 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 5 | 0.48 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 5 | 0.48 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 5 | 0.48 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 16 | 0.48 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 16 | 0.48 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 16 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 5 | 0.48 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 5 | 0.48 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 2 | 0.48 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 4 | 0.48 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 16 | 0.48 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 16 | 0.48 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 16 | 0.48 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 9 | 0.48 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 9 | 0.48 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 9 | 0.48 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 5 | 0.48 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 5 | 0.48 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 5 | 0.48 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 9 | 0.48 |
| (1,1219) | 1:169:A:THR:HG21 | 1:171:A:ASP:H | 3 | 0.48 |
| (1,1219) | 1:169:A:THR:HG22 | 1:171:A:ASP:H | 3 | 0.48 |
| (1,1219) | 1:169:A:THR:HG23 | 1:171:A:ASP:H | 3 | 0.48 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 8 | 0.48 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 6 | 0.48 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 13 | 0.48 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 13 | 0.48 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 13 | 0.48 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 13 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 4 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 4 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 4 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 15 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 15 | 0.48 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 15 | 0.48 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 10 | 0.48 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 10 | 0.48 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 10 | 0.48 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG21 | 20 | 0.48 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG22 | 20 | 0.48 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG23 | 20 | 0.48 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 11 | 0.48 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 11 | 0.48 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 13 | 0.48 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 13 | 0.48 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 13 | 0.48 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 11 | 0.48 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 11 | 0.48 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 16 | 0.48 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 16 | 0.48 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 1 | 0.48 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 10 | 0.48 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 10 | 0.48 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 10 | 0.48 |
| (1,572) | 1:92:A:LYS:HD2 | 1:93:A:GLU:H | 7 | 0.48 |
| (1,572) | 1:92:A:LYS:HD3 | 1:93:A:GLU:H | 7 | 0.48 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 12 | 0.48 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 7 | 0.48 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 8 | 0.48 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 8 | 0.48 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 9 | 0.48 |
| (1,414) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HA | 16 | 0.48 |
| (1,414) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HA | 16 | 0.48 |
| (1,414) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HA | 16 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 4 | 0.48 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 4 | 0.48 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 4 | 0.48 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 9 | 0.48 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 9 | 0.48 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 9 | 0.48 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 12 | 0.48 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 12 | 0.48 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 12 | 0.48 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 19 | 0.48 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 19 | 0.48 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 19 | 0.48 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 4 | 0.48 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 14 | 0.48 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 14 | 0.48 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 14 | 0.48 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE1 | 5 | 0.48 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE2 | 5 | 0.48 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 16 | 0.47 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 16 | 0.47 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 16 | 0.47 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 16 | 0.47 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 20 | 0.47 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 20 | 0.47 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 20 | 0.47 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 20 | 0.47 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 20 | 0.47 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 20 | 0.47 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 14 | 0.47 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 14 | 0.47 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 14 | 0.47 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 14 | 0.47 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 14 | 0.47 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 14 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 10 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 10 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 10 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 10 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 10 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 10 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 13 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 13 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 13 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 13 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 13 | 0.47 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 13 | 0.47 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG2 | 15 | 0.47 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG3 | 15 | 0.47 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 5 | 0.47 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 5 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 4 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 4 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 4 | 0.47 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 4 | 0.47 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 14 | 0.47 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 14 | 0.47 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 14 | 0.47 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 8 | 0.47 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 8 | 0.47 |
| (1,3396) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HA | 7 | 0.47 |
| (1,3396) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HA | 7 | 0.47 |
| (1,3396) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HA | 7 | 0.47 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 20 | 0.47 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 20 | 0.47 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 20 | 0.47 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 20 | 0.47 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 12 | 0.47 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 18 | 0.47 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 12 | 0.47 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 12 | 0.47 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 10 | 0.47 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 10 | 0.47 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 10 | 0.47 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 16 | 0.47 |
| (1,3204) | 1:88:A:GLN:HB3 | 1:90:A:HIS:HE1 | 3 | 0.47 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 1 | 0.47 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 1 | 0.47 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 1 | 0.47 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 11 | 0.47 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 5 | 0.47 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 12 | 0.47 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 12 | 0.47 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 2 | 0.47 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 4 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 20 | 0.47 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 1 | 0.47 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 8 | 0.47 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 15 | 0.47 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 16 | 0.47 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 18 | 0.47 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 20 | 0.47 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 20 | 0.47 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 20 | 0.47 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 5 | 0.47 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 17 | 0.47 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 17 | 0.47 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 17 | 0.47 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 12 | 0.47 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 12 | 0.47 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 12 | 0.47 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 18 | 0.47 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 18 | 0.47 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 18 | 0.47 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 16 | 0.47 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 11 | 0.47 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 11 | 0.47 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 11 | 0.47 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 9 | 0.47 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 10 | 0.47 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD1 | 17 | 0.47 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD2 | 17 | 0.47 |
| (1,2303) | 1:77:A:GLN:HB2 | 1:80:A:SER:H | 6 | 0.47 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 6 | 0.47 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 16 | 0.47 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 8 | 0.47 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 8 | 0.47 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 8 | 0.47 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 13 | 0.47 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 4 | 0.47 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 4 | 0.47 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 4 | 0.47 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 4 | 0.47 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 4 | 0.47 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 4 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 1 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 1 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 10 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 11 | 0.47 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 11 | 0.47 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 1 | 0.47 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE2 | 12 | 0.47 |
| (1,1784) | 1:200:A:ALA:HB1 | 1:205:A:LYS:HE3 | 12 | 0.47 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE2 | 12 | 0.47 |
| (1,1784) | 1:200:A:ALA:HB2 | 1:205:A:LYS:HE3 | 12 | 0.47 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE2 | 12 | 0.47 |
| (1,1784) | 1:200:A:ALA:HB3 | 1:205:A:LYS:HE3 | 12 | 0.47 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 12 | 0.47 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 12 | 0.47 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 5 | 0.47 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 13 | 0.47 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 1 | 0.47 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 10 | 0.47 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 7 | 0.47 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 7 | 0.47 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 7 | 0.47 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 3 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 3 | 0.47 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 3 | 0.47 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 11 | 0.47 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 11 | 0.47 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 11 | 0.47 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 11 | 0.47 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 18 | 0.47 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 18 | 0.47 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 18 | 0.47 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 14 | 0.47 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 14 | 0.47 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 14 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 18 | 0.47 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 18 | 0.47 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 4 | 0.47 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 12 | 0.47 |
| (1,1441) | 1:142:A:THR:HG21 | 1:178:A:ALA:HA | 19 | 0.47 |
| (1,1441) | 1:142:A:THR:HG22 | 1:178:A:ALA:HA | 19 | 0.47 |
| (1,1441) | 1:142:A:THR:HG23 | 1:178:A:ALA:HA | 19 | 0.47 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 5 | 0.47 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 5 | 0.47 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 5 | 0.47 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 5 | 0.47 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 5 | 0.47 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 9 | 0.47 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 9 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 11 | 0.47 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 2 | 0.47 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 3 | 0.47 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 3 | 0.47 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 3 | 0.47 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 20 | 0.47 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 15 | 0.47 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 15 | 0.47 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 15 | 0.47 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 11 | 0.47 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 11 | 0.47 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 11 | 0.47 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 9 | 0.47 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 9 | 0.47 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 9 | 0.47 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 16 | 0.47 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 16 | 0.47 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 16 | 0.47 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 16 | 0.47 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 16 | 0.47 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 16 | 0.47 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 1 | 0.47 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 1 | 0.47 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 1 | 0.47 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 6 | 0.47 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 6 | 0.47 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 13 | 0.47 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 7 | 0.47 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 7 | 0.47 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 7 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 6 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 6 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 6 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 7 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 7 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 7 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 12 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 12 | 0.47 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 12 | 0.47 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 9 | 0.47 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 9 | 0.47 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 9 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 17 | 0.47 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 14 | 0.47 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 13 | 0.47 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 6 | 0.47 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 6 | 0.47 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 6 | 0.47 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 6 | 0.47 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 6 | 0.47 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 6 | 0.47 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 14 | 0.47 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 14 | 0.47 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 14 | 0.47 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 3 | 0.47 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 3 | 0.47 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 2 | 0.47 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 5 | 0.47 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 5 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 8 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 8 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 8 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 8 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 8 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 8 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 9 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 9 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 9 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 9 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 9 | 0.47 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 9 | 0.47 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 7 | 0.47 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 7 | 0.47 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 7 | 0.47 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 3 | 0.47 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 4 | 0.47 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 4 | 0.47 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 4 | 0.47 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 4 | 0.47 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 4 | 0.47 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 4 | 0.47 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 7 | 0.47 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 7 | 0.47 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 7 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 3 | 0.47 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 3 | 0.47 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 3 | 0.47 |
| (1,284) | 1:60:A:LYS:HE3 | 1:68:A:VAL:HG11 | 17 | 0.47 |
| (1,284) | 1:60:A:LYS:HE3 | 1:68:A:VAL:HG12 | 17 | 0.47 |
| (1,284) | 1:60:A:LYS:HE3 | 1:68:A:VAL:HG13 | 17 | 0.47 |
| (1,284) | 1:60:A:LYS:HE3 | 1:68:A:VAL:HG21 | 17 | 0.47 |
| (1,284) | 1:60:A:LYS:HE3 | 1:68:A:VAL:HG22 | 17 | 0.47 |
| (1,284) | 1:60:A:LYS:HE3 | 1:68:A:VAL:HG23 | 17 | 0.47 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 1 | 0.47 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 1 | 0.47 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 1 | 0.47 |
| (1,68) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG2 | 6 | 0.47 |
| (1,68) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG2 | 6 | 0.47 |
| (1,68) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG2 | 6 | 0.47 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 8 | 0.47 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 14 | 0.47 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 13 | 0.47 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 13 | 0.47 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 13 | 0.47 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 12 | 0.46 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 12 | 0.46 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 16 | 0.46 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 16 | 0.46 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 3 | 0.46 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 3 | 0.46 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 17 | 0.46 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 17 | 0.46 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG11 | 7 | 0.46 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG12 | 7 | 0.46 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG13 | 7 | 0.46 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG21 | 7 | 0.46 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG22 | 7 | 0.46 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG23 | 7 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 4 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 4 | 0.46 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 4 | 0.46 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 17 | 0.46 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 17 | 0.46 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 17 | 0.46 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 17 | 0.46 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 17 | 0.46 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 17 | 0.46 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 18 | 0.46 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 18 | 0.46 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 18 | 0.46 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 18 | 0.46 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 18 | 0.46 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 18 | 0.46 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 16 | 0.46 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 16 | 0.46 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG21 | 3 | 0.46 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG22 | 3 | 0.46 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG23 | 3 | 0.46 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG21 | 3 | 0.46 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG22 | 3 | 0.46 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG23 | 3 | 0.46 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD21 | 11 | 0.46 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD22 | 11 | 0.46 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD21 | 11 | 0.46 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD22 | 11 | 0.46 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG2 | 17 | 0.46 |
| (1,3661) | 1:89:A:LEU:HG | 1:91:A:GLN:HG3 | 17 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 16 | 0.46 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 16 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 13 | 0.46 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 13 | 0.46 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 16 | 0.46 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 15 | 0.46 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 5 | 0.46 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 5 | 0.46 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 5 | 0.46 |
| (1,3429) | 2:4:B:LYS:HA | 2:4:B:LYS:HD2 | 3 | 0.46 |
| (1,3429) | 2:4:B:LYS:HA | 2:4:B:LYS:HD3 | 3 | 0.46 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 20 | 0.46 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 20 | 0.46 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 3 | 0.46 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 3 | 0.46 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 15 | 0.46 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 15 | 0.46 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 14 | 0.46 |
| (1,3208) | 1:126:A:ALA:HB1 | 1:133:A:TRP:HD1 | 9 | 0.46 |
| (1,3208) | 1:126:A:ALA:HB2 | 1:133:A:TRP:HD1 | 9 | 0.46 |
| (1,3208) | 1:126:A:ALA:HB3 | 1:133:A:TRP:HD1 | 9 | 0.46 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 14 | 0.46 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 14 | 0.46 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 14 | 0.46 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 8 | 0.46 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 14 | 0.46 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 11 | 0.46 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 18 | 0.46 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 12 | 0.46 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 5 | 0.46 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 14 | 0.46 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 2 | 0.46 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 6 | 0.46 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 19 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 15 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 15 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 15 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 19 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 19 | 0.46 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 19 | 0.46 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 14 | 0.46 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 20 | 0.46 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 18 | 0.46 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 14 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 11 | 0.46 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 17 | 0.46 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 1 | 0.46 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 20 | 0.46 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 15 | 0.46 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 19 | 0.46 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 7 | 0.46 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 6 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 13 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 13 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 13 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 18 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 18 | 0.46 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 18 | 0.46 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 12 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 7 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 19 | 0.46 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 19 | 0.46 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 12 | 0.46 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 12 | 0.46 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG21 | 8 | 0.46 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG22 | 8 | 0.46 |
| (1,1820) | 1:170:A:PHE:HB2 | 1:201:A:ILE:HG23 | 8 | 0.46 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 3 | 0.46 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 3 | 0.46 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 3 | 0.46 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 2 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 2 | 0.46 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 2 | 0.46 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 6 | 0.46 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 6 | 0.46 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 6 | 0.46 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 6 | 0.46 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 6 | 0.46 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 6 | 0.46 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 18 | 0.46 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 16 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 10 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 10 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 10 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 16 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 16 | 0.46 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 16 | 0.46 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 20 | 0.46 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 7 | 0.46 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 10 | 0.46 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 10 | 0.46 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 10 | 0.46 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 10 | 0.46 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 10 | 0.46 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 10 | 0.46 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 4 | 0.46 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 4 | 0.46 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 4 | 0.46 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 4 | 0.46 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 4 | 0.46 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 4 | 0.46 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 14 | 0.46 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 2 | 0.46 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 7 | 0.46 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 20 | 0.46 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 19 | 0.46 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 6 | 0.46 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 11 | 0.46 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 14 | 0.46 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 20 | 0.46 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 10 | 0.46 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 10 | 0.46 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 10 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,676) | 1:103:A:THR:HG21 | 1:128:A:LEU:H | 5 | 0.46 |
| (1,676) | 1:103:A:THR:HG22 | 1:128:A:LEU:H | 5 | 0.46 |
| (1,676) | 1:103:A:THR:HG23 | 1:128:A:LEU:H | 5 | 0.46 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 18 | 0.46 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 18 | 0.46 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 18 | 0.46 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG11 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG12 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG13 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG21 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG22 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG23 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG11 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG12 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG13 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG21 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG22 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG23 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG11 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG12 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG13 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG21 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG22 | 8 | 0.46 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG23 | 8 | 0.46 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 3 | 0.46 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 16 | 0.46 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 20 | 0.46 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 20 | 0.46 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 20 | 0.46 |
| (1,386) | 1:75:A:ILE:HD11 | 1:84:A:ALA:H | 8 | 0.46 |
| (1,386) | 1:75:A:ILE:HD12 | 1:84:A:ALA:H | 8 | 0.46 |
| (1,386) | 1:75:A:ILE:HD13 | 1:84:A:ALA:H | 8 | 0.46 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 10 | 0.46 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 10 | 0.46 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 10 | 0.46 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 6 | 0.46 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 6 | 0.46 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 6 | 0.46 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 8 | 0.46 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 11 | 0.46 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 1 | 0.46 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 1 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 1 | 0.46 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 14 | 0.46 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 14 | 0.46 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 14 | 0.46 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 11 | 0.46 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 11 | 0.46 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 11 | 0.46 |
| (1,81) | 1:52:A:VAL:HG11 | 1:53:A:THR:HB | 18 | 0.46 |
| (1,81) | 1:52:A:VAL:HG12 | 1:53:A:THR:HB | 18 | 0.46 |
| (1,81) | 1:52:A:VAL:HG13 | 1:53:A:THR:HB | 18 | 0.46 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 13 | 0.45 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 13 | 0.45 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 18 | 0.45 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 18 | 0.45 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 15 | 0.45 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 15 | 0.45 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG11 | 9 | 0.45 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG12 | 9 | 0.45 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG13 | 9 | 0.45 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG21 | 9 | 0.45 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG22 | 9 | 0.45 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG23 | 9 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 14 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 14 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 14 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 14 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 14 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 14 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 17 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 17 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 17 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 17 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 17 | 0.45 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 17 | 0.45 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 15 | 0.45 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 15 | 0.45 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 15 | 0.45 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 15 | 0.45 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 15 | 0.45 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 15 | 0.45 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 8 | 0.45 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 8 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 8 | 0.45 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 8 | 0.45 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 8 | 0.45 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 8 | 0.45 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 6 | 0.45 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 6 | 0.45 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 13 | 0.45 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 13 | 0.45 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 13 | 0.45 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 13 | 0.45 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 13 | 0.45 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 13 | 0.45 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 17 | 0.45 |
| (1,3570) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 17 | 0.45 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 17 | 0.45 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 17 | 0.45 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 17 | 0.45 |
| (1,3490) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HB | 16 | 0.45 |
| (1,3490) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HB | 16 | 0.45 |
| (1,3490) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HB | 16 | 0.45 |
| (1,3486) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HA | 2 | 0.45 |
| (1,3486) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HA | 2 | 0.45 |
| (1,3486) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HA | 2 | 0.45 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 11 | 0.45 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 11 | 0.45 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 11 | 0.45 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 11 | 0.45 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 11 | 0.45 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 11 | 0.45 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 11 | 0.45 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 11 | 0.45 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 11 | 0.45 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 9 | 0.45 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 11 | 0.45 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 11 | 0.45 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 11 | 0.45 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 17 | 0.45 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 12 | 0.45 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 12 | 0.45 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 19 | 0.45 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 19 | 0.45 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 19 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 4 | 0.45 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 4 | 0.45 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 4 | 0.45 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 14 | 0.45 |
| (1,3011) | 1:215:A:GLU:HG2 | 1:217:A:GLY:H | 2 | 0.45 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 10 | 0.45 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 10 | 0.45 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 10 | 0.45 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 3 | 0.45 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 11 | 0.45 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 20 | 0.45 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 17 | 0.45 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 13 | 0.45 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 13 | 0.45 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 13 | 0.45 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 14 | 0.45 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 14 | 0.45 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 14 | 0.45 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 2 | 0.45 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 2 | 0.45 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 2 | 0.45 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 2 | 0.45 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 2 | 0.45 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 2 | 0.45 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 3 | 0.45 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 19 | 0.45 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 19 | 0.45 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 19 | 0.45 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 20 | 0.45 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 20 | 0.45 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 20 | 0.45 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 9 | 0.45 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 9 | 0.45 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 9 | 0.45 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 16 | 0.45 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 15 | 0.45 |
| (1,2217) | 1:62:A:ASP:H | 1:66:A:ASP:HB2 | 5 | 0.45 |
| (1,2142) | 1:47:A:THR:HB | 1:50:A:LEU:H | 16 | 0.45 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 9 | 0.45 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 9 | 0.45 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 9 | 0.45 |
| (1,2123) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 3 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 15 | 0.45 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 15 | 0.45 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 6 | 0.45 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 9 | 0.45 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 20 | 0.45 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 19 | 0.45 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 20 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 6 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 6 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 6 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 16 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 16 | 0.45 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 16 | 0.45 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 17 | 0.45 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 11 | 0.45 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 11 | 0.45 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 11 | 0.45 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 5 | 0.45 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 1 | 0.45 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 4 | 0.45 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 4 | 0.45 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 18 | 0.45 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 18 | 0.45 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 18 | 0.45 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 6 | 0.45 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 5 | 0.45 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 5 | 0.45 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 4 | 0.45 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 4 | 0.45 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 4 | 0.45 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 3 | 0.45 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 4 | 0.45 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 13 | 0.45 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 17 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD11 | 3 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD12 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD13 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD21 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD22 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB1 | 1:179:A:LEU:HD23 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD11 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD12 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD13 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD21 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD22 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB2 | 1:179:A:LEU:HD23 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD11 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD12 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD13 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD21 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD22 | 3 | 0.45 |
| (1,1462) | 1:178:A:ALA:HB3 | 1:179:A:LEU:HD23 | 3 | 0.45 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 16 | 0.45 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 14 | 0.45 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 3 | 0.45 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 4 | 0.45 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 4 | 0.45 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 4 | 0.45 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 9 | 0.45 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 9 | 0.45 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 9 | 0.45 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 11 | 0.45 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 17 | 0.45 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 17 | 0.45 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 17 | 0.45 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 17 | 0.45 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 17 | 0.45 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 17 | 0.45 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 6 | 0.45 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 6 | 0.45 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 1 | 0.45 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 1 | 0.45 |
| (1,1161) | 1:147:A:GLY:HA2 | 1:148:A:SER:HB2 | 19 | 0.45 |
| (1,1161) | 1:147:A:GLY:HA2 | 1:148:A:SER:HB3 | 19 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 1 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 1 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 1 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 3 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 3 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 3 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 13 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 13 | 0.45 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 13 | 0.45 |
| (1,1127) | 1:117:A:VAL:HA | 1:143:A:VAL:HA | 19 | 0.45 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 11 | 0.45 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 11 | 0.45 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 11 | 0.45 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 15 | 0.45 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 15 | 0.45 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 15 | 0.45 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 17 | 0.45 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 17 | 0.45 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 10 | 0.45 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 4 | 0.45 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 4 | 0.45 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 4 | 0.45 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 14 | 0.45 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 14 | 0.45 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 14 | 0.45 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 2 | 0.45 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 13 | 0.45 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 10 | 0.45 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 19 | 0.45 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 19 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 20 | 0.45 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 16 | 0.45 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 16 | 0.45 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 16 | 0.45 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 16 | 0.45 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 3 | 0.45 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 3 | 0.45 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 3 | 0.45 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 13 | 0.45 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 13 | 0.45 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 13 | 0.45 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 16 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 6 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 6 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 6 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 15 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 15 | 0.45 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 15 | 0.45 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 13 | 0.45 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 13 | 0.45 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 13 | 0.45 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 15 | 0.45 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 1 | 0.45 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 18 | 0.45 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 6 | 0.45 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 6 | 0.45 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 6 | 0.45 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 15 | 0.45 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 19 | 0.45 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 2 | 0.45 |
| (1,196) | 1:167:A:ASP:HA | 1:196:A:ASN:HB2 | 19 | 0.45 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 1 | 0.45 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 1 | 0.45 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 1 | 0.45 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 11 | 0.45 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 11 | 0.45 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 11 | 0.45 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 18 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 18 | 0.45 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 18 | 0.45 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 5 | 0.45 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 5 | 0.45 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 5 | 0.45 |
| (1,3949) | 1:193:A:THR:HB | 1:195:A:ASN:HD21 | 2 | 0.44 |
| (1,3949) | 1:193:A:THR:HB | 1:195:A:ASN:HD22 | 2 | 0.44 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 8 | 0.44 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 8 | 0.44 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 19 | 0.44 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 19 | 0.44 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 2 | 0.44 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 2 | 0.44 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 2 | 0.44 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 2 | 0.44 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 2 | 0.44 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 2 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 1 | 0.44 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 1 | 0.44 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 16 | 0.44 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 16 | 0.44 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 16 | 0.44 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 16 | 0.44 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 16 | 0.44 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 16 | 0.44 |
| (1,3845) | 1:138:A:ALA:HA | 1:150:A:SER:HB2 | 10 | 0.44 |
| (1,3845) | 1:138:A:ALA:HA | 1:150:A:SER:HB3 | 10 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 19 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 19 | 0.44 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 19 | 0.44 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 4 | 0.44 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 4 | 0.44 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG2 | 4 | 0.44 |
| (1,3684) | 1:94:A:ALA:HA | 1:97:A:GLN:HG3 | 4 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE21 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HE22 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE21 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HE22 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE21 | 17 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3664) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HE22 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE21 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HE22 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE21 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HE22 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE21 | 17 | 0.44 |
| (1,3664) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HE22 | 17 | 0.44 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 16 | 0.44 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 16 | 0.44 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 4 | 0.44 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 4 | 0.44 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 4 | 0.44 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 4 | 0.44 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 4 | 0.44 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 4 | 0.44 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 9 | 0.44 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 13 | 0.44 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 13 | 0.44 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 13 | 0.44 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 13 | 0.44 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 13 | 0.44 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 13 | 0.44 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 3 | 0.44 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 3 | 0.44 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 3 | 0.44 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 14 | 0.44 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 14 | 0.44 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 14 | 0.44 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 7 | 0.44 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 7 | 0.44 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 7 | 0.44 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 13 | 0.44 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 13 | 0.44 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 1 | 0.44 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 1 | 0.44 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 1 | 0.44 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 1 | 0.44 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 12 | 0.44 |
| (1,3274) | 1:111:A:HIS:HD2 | 1:113:A:ASP:H | 7 | 0.44 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 3 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 3 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 3 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 3 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 14 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 14 | 0.44 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 14 | 0.44 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 18 | 0.44 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 18 | 0.44 |
| (1,3208) | 1:126:A:ALA:HB1 | 1:133:A:TRP:HD1 | 3 | 0.44 |
| (1,3208) | 1:126:A:ALA:HB2 | 1:133:A:TRP:HD1 | 3 | 0.44 |
| (1,3208) | 1:126:A:ALA:HB3 | 1:133:A:TRP:HD1 | 3 | 0.44 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 6 | 0.44 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 6 | 0.44 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 20 | 0.44 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 7 | 0.44 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 15 | 0.44 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 17 | 0.44 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 20 | 0.44 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 19 | 0.44 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 18 | 0.44 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB2 | 15 | 0.44 |
| (1,3006) | 1:214:A:ALA:H | 1:215:A:GLU:HB3 | 15 | 0.44 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 4 | 0.44 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 19 | 0.44 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 10 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 3 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 4 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 6 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 8 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 13 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 16 | 0.44 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 17 | 0.44 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 16 | 0.44 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 16 | 0.44 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 16 | 0.44 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 6 | 0.44 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 2 | 0.44 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 5 | 0.44 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 7 | 0.44 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 10 | 0.44 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 17 | 0.44 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 13 | 0.44 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 3 | 0.44 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 17 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 20 | 0.44 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 20 | 0.44 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 11 | 0.44 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 12 | 0.44 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 13 | 0.44 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 3 | 0.44 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 18 | 0.44 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 4 | 0.44 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 16 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 14 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 14 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 14 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 15 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 15 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 15 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 19 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 19 | 0.44 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 19 | 0.44 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 5 | 0.44 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 13 | 0.44 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 8 | 0.44 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 8 | 0.44 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 8 | 0.44 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 15 | 0.44 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 13 | 0.44 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 3 | 0.44 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 3 | 0.44 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 3 | 0.44 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 3 | 0.44 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 3 | 0.44 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 3 | 0.44 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 6 | 0.44 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 6 | 0.44 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 6 | 0.44 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 17 | 0.44 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 17 | 0.44 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 17 | 0.44 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 11 | 0.44 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 11 | 0.44 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 11 | 0.44 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 17 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 7 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 7 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 7 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 12 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 12 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 12 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 19 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 19 | 0.44 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 19 | 0.44 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 1 | 0.44 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 1 | 0.44 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 1 | 0.44 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 15 | 0.44 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 15 | 0.44 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 15 | 0.44 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 1 | 0.44 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 14 | 0.44 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 10 | 0.44 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 11 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 12 | 0.44 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 12 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 11 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 11 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 11 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 11 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 12 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 12 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 12 | 0.44 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 12 | 0.44 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 12 | 0.44 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG21 | 3 | 0.44 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG22 | 3 | 0.44 |
| (1,1239) | 1:153:A:VAL:H | 1:154:A:ILE:HG23 | 3 | 0.44 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 3 | 0.44 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 17 | 0.44 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 10 | 0.44 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 10 | 0.44 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 10 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 2 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 2 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 2 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 4 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 4 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 4 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 8 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 8 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 8 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 10 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 10 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 10 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 14 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 14 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 14 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 17 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 17 | 0.44 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 17 | 0.44 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 8 | 0.44 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 11 | 0.44 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 11 | 0.44 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 11 | 0.44 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 18 | 0.44 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 18 | 0.44 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 18 | 0.44 |
| (1,1052) | 1:139:A:SER:HB3 | 1:149:A:ALA:H | 18 | 0.44 |
| (1,998) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HA | 4 | 0.44 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG11 | 20 | 0.44 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG12 | 20 | 0.44 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG13 | 20 | 0.44 |
| (1,938) | 1:103:A:THR:HA | 1:128:A:LEU:HG | 20 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,932) | 1:128:A:LEU:HA | 1:128:A:LEU:HD11 | 5 | 0.44 |
| (1,932) | 1:128:A:LEU:HA | 1:128:A:LEU:HD12 | 5 | 0.44 |
| (1,932) | 1:128:A:LEU:HA | 1:128:A:LEU:HD13 | 5 | 0.44 |
| (1,932) | 1:128:A:LEU:HA | 1:128:A:LEU:HD21 | 5 | 0.44 |
| (1,932) | 1:128:A:LEU:HA | 1:128:A:LEU:HD22 | 5 | 0.44 |
| (1,932) | 1:128:A:LEU:HA | 1:128:A:LEU:HD23 | 5 | 0.44 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 16 | 0.44 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 16 | 0.44 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 16 | 0.44 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 13 | 0.44 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 17 | 0.44 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 18 | 0.44 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 18 | 0.44 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 11 | 0.44 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 11 | 0.44 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 18 | 0.44 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 18 | 0.44 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 19 | 0.44 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 19 | 0.44 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 19 | 0.44 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 19 | 0.44 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 19 | 0.44 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 19 | 0.44 |
| (1,569) | 1:52:A:VAL:HA | 1:76:A:MET:HB3 | 10 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 2 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 2 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 2 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 18 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 18 | 0.44 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 18 | 0.44 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 9 | 0.44 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 4 | 0.44 |
| (1,465) | 1:81:A:ARG:H | 1:81:A:ARG:HD3 | 18 | 0.44 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 3 | 0.44 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 20 | 0.44 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 20 | 0.44 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 17 | 0.44 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 17 | 0.44 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 17 | 0.44 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 19 | 0.44 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 19 | 0.44 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 19 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 10 | 0.44 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 12 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 4 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 4 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 4 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 12 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 12 | 0.44 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 12 | 0.44 |
| (1,68) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG2 | 3 | 0.44 |
| (1,68) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG2 | 3 | 0.44 |
| (1,68) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG2 | 3 | 0.44 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 14 | 0.44 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 14 | 0.44 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 14 | 0.44 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 14 | 0.44 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 14 | 0.44 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 14 | 0.44 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 5 | 0.43 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 5 | 0.43 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 5 | 0.43 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 5 | 0.43 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 5 | 0.43 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 5 | 0.43 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 11 | 0.43 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 11 | 0.43 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 11 | 0.43 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 11 | 0.43 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 11 | 0.43 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 11 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 13 | 0.43 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 13 | 0.43 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 1 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 1 | 0.43 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 14 | 0.43 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 14 | 0.43 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 14 | 0.43 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 14 | 0.43 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 12 | 0.43 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 12 | 0.43 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 14 | 0.43 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 5 | 0.43 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 5 | 0.43 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 9 | 0.43 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 9 | 0.43 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 9 | 0.43 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 19 | 0.43 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 19 | 0.43 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 19 | 0.43 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 11 | 0.43 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 11 | 0.43 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 11 | 0.43 |
| (1,3476) | 2:10:B:TYR:HE1 | 2:21:B:MET:HB3 | 7 | 0.43 |
| (1,3476) | 2:10:B:TYR:HE2 | 2:21:B:MET:HB3 | 7 | 0.43 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 1 | 0.43 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 1 | 0.43 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 1 | 0.43 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG21 | 17 | 0.43 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG22 | 17 | 0.43 |
| (1,3391) | 2:12:B:ASN:HD22 | 2:15:B:THR:HG23 | 17 | 0.43 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 11 | 0.43 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 11 | 0.43 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 6 | 0.43 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 6 | 0.43 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 10 | 0.43 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 10 | 0.43 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 1 | 0.43 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 1 | 0.43 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 1 | 0.43 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 17 | 0.43 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 3 | 0.43 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 10 | 0.43 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 14 | 0.43 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 15 | 0.43 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 15 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 15 | 0.43 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 15 | 0.43 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 11 | 0.43 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 7 | 0.43 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 7 | 0.43 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 7 | 0.43 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 9 | 0.43 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 9 | 0.43 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 9 | 0.43 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 5 | 0.43 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 14 | 0.43 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 11 | 0.43 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 11 | 0.43 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 14 | 0.43 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 12 | 0.43 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 11 | 0.43 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 13 | 0.43 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 15 | 0.43 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 20 | 0.43 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 3 | 0.43 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 3 | 0.43 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 3 | 0.43 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 3 | 0.43 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 3 | 0.43 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 3 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 20 | 0.43 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 20 | 0.43 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 6 | 0.43 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 6 | 0.43 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 6 | 0.43 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 13 | 0.43 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 5 | 0.43 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 16 | 0.43 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 15 | 0.43 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 15 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 15 | 0.43 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 1 | 0.43 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 19 | 0.43 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 3 | 0.43 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 3 | 0.43 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 3 | 0.43 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 20 | 0.43 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 20 | 0.43 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 20 | 0.43 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 12 | 0.43 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 6 | 0.43 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 6 | 0.43 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 3 | 0.43 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 12 | 0.43 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 12 | 0.43 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 12 | 0.43 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD11 | 12 | 0.43 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD12 | 12 | 0.43 |
| (1,1491) | 1:179:A:LEU:H | 1:180:A:ILE:HD13 | 12 | 0.43 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 8 | 0.43 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 17 | 0.43 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 19 | 0.43 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 6 | 0.43 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 6 | 0.43 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 6 | 0.43 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 9 | 0.43 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 9 | 0.43 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 9 | 0.43 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 18 | 0.43 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 18 | 0.43 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 18 | 0.43 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 18 | 0.43 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 19 | 0.43 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 4 | 0.43 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 4 | 0.43 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 4 | 0.43 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 4 | 0.43 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 4 | 0.43 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 4 | 0.43 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 4 | 0.43 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 7 | 0.43 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 7 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 7 | 0.43 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 5 | 0.43 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 5 | 0.43 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 5 | 0.43 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 7 | 0.43 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 7 | 0.43 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 7 | 0.43 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 15 | 0.43 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 13 | 0.43 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 8 | 0.43 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 8 | 0.43 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 7 | 0.43 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 2 | 0.43 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 2 | 0.43 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 2 | 0.43 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 20 | 0.43 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 20 | 0.43 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 20 | 0.43 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 3 | 0.43 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 3 | 0.43 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 3 | 0.43 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 10 | 0.43 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 10 | 0.43 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 10 | 0.43 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 4 | 0.43 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 7 | 0.43 |
| (1,728) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HD3 | 11 | 0.43 |
| (1,728) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HD3 | 11 | 0.43 |
| (1,728) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HD3 | 11 | 0.43 |
| (1,728) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HD3 | 11 | 0.43 |
| (1,728) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HD3 | 11 | 0.43 |
| (1,728) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HD3 | 11 | 0.43 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD11 | 13 | 0.43 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD12 | 13 | 0.43 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD13 | 13 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD21 | 13 | 0.43 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD22 | 13 | 0.43 |
| (1,659) | 1:103:A:THR:HA | 1:128:A:LEU:HD23 | 13 | 0.43 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 5 | 0.43 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 5 | 0.43 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 9 | 0.43 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 9 | 0.43 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 9 | 0.43 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 9 | 0.43 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 9 | 0.43 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 9 | 0.43 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 1 | 0.43 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 1 | 0.43 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 1 | 0.43 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 8 | 0.43 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 8 | 0.43 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 8 | 0.43 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 2 | 0.43 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 2 | 0.43 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 2 | 0.43 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 7 | 0.43 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 7 | 0.43 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 7 | 0.43 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 17 | 0.43 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 17 | 0.43 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 17 | 0.43 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 7 | 0.43 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG21 | 20 | 0.43 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG22 | 20 | 0.43 |
| (1,366) | 1:58:A:HIS:HB3 | 1:73:A:VAL:HG23 | 20 | 0.43 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 7 | 0.43 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 7 | 0.43 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 7 | 0.43 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 4 | 0.43 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 4 | 0.43 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 4 | 0.43 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 11 | 0.43 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 4 | 0.43 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 4 | 0.43 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 4 | 0.43 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 12 | 0.42 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 12 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 7 | 0.42 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 7 | 0.42 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 7 | 0.42 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 7 | 0.42 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 7 | 0.42 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 7 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 5 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 5 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 5 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 5 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 5 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 5 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 6 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 6 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 6 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 6 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 6 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 6 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 18 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 18 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 18 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 18 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 18 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 18 | 0.42 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 12 | 0.42 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 12 | 0.42 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 12 | 0.42 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 12 | 0.42 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 12 | 0.42 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 12 | 0.42 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG11 | 11 | 0.42 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG12 | 11 | 0.42 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG13 | 11 | 0.42 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG21 | 11 | 0.42 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG22 | 11 | 0.42 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG23 | 11 | 0.42 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 8 | 0.42 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 8 | 0.42 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 14 | 0.42 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 14 | 0.42 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 15 | 0.42 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 15 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 6 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 6 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 6 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 6 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 6 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 6 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 17 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 17 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 17 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 17 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 17 | 0.42 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 17 | 0.42 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 11 | 0.42 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 11 | 0.42 |
| (1,3654) | 1:88:A:GLN:HG2 | 1:90:A:HIS:HE1 | 8 | 0.42 |
| (1,3654) | 1:88:A:GLN:HG3 | 1:90:A:HIS:HE1 | 8 | 0.42 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 7 | 0.42 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 7 | 0.42 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 7 | 0.42 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 7 | 0.42 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 7 | 0.42 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 7 | 0.42 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB2 | 20 | 0.42 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB3 | 20 | 0.42 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB2 | 20 | 0.42 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB3 | 20 | 0.42 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB2 | 20 | 0.42 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB3 | 20 | 0.42 |
| (1,3497) | 1:67:A:ALA:HB1 | 2:21:B:MET:HB2 | 8 | 0.42 |
| (1,3497) | 1:67:A:ALA:HB2 | 2:21:B:MET:HB2 | 8 | 0.42 |
| (1,3497) | 1:67:A:ALA:HB3 | 2:21:B:MET:HB2 | 8 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 15 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 15 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 15 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 15 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 15 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 15 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 16 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 16 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 16 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 16 | 0.42 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 16 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 16 | 0.42 |
| (1,3429) | 2:4:B:LYS:HA | 2:4:B:LYS:HD2 | 15 | 0.42 |
| (1,3429) | 2:4:B:LYS:HA | 2:4:B:LYS:HD3 | 15 | 0.42 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 16 | 0.42 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 16 | 0.42 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 16 | 0.42 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD2 | 20 | 0.42 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD3 | 20 | 0.42 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 17 | 0.42 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 17 | 0.42 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 19 | 0.42 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 19 | 0.42 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 19 | 0.42 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 20 | 0.42 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 20 | 0.42 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 20 | 0.42 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 3 | 0.42 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 3 | 0.42 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 3 | 0.42 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 14 | 0.42 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 14 | 0.42 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 14 | 0.42 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 5 | 0.42 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 5 | 0.42 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 11 | 0.42 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 1 | 0.42 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG11 | 12 | 0.42 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG12 | 12 | 0.42 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG13 | 12 | 0.42 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG11 | 12 | 0.42 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG12 | 12 | 0.42 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG13 | 12 | 0.42 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 2 | 0.42 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 3 | 0.42 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 4 | 0.42 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 7 | 0.42 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 17 | 0.42 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 2 | 0.42 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 2 | 0.42 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 2 | 0.42 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 15 | 0.42 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 4 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 4 | 0.42 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 4 | 0.42 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 7 | 0.42 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 7 | 0.42 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 7 | 0.42 |
| (1,2626) | 1:145:A:ALA:H | 1:182:A:HIS:HE1 | 9 | 0.42 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 3 | 0.42 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 8 | 0.42 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 2 | 0.42 |
| (1,2437) | 1:82:A:LEU:HG | 1:113:A:ASP:H | 18 | 0.42 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 18 | 0.42 |
| (1,2210) | 1:60:A:LYS:H | 1:60:A:LYS:HE2 | 17 | 0.42 |
| (1,2189) | 1:58:A:HIS:H | 2:12:B:ASN:HD21 | 5 | 0.42 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 19 | 0.42 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 19 | 0.42 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 19 | 0.42 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 20 | 0.42 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 20 | 0.42 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 1 | 0.42 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 2 | 0.42 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 9 | 0.42 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 15 | 0.42 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 18 | 0.42 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 8 | 0.42 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 10 | 0.42 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 18 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 1 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 1 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 1 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 8 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 8 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 8 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 9 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 9 | 0.42 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 9 | 0.42 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 6 | 0.42 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 6 | 0.42 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 6 | 0.42 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 17 | 0.42 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 9 | 0.42 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 9 | 0.42 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 9 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 8 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 7 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 7 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 7 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 17 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 17 | 0.42 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 17 | 0.42 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 4 | 0.42 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 15 | 0.42 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 15 | 0.42 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 15 | 0.42 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 14 | 0.42 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 14 | 0.42 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 14 | 0.42 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 17 | 0.42 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 17 | 0.42 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 17 | 0.42 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 20 | 0.42 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 20 | 0.42 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 20 | 0.42 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 5 | 0.42 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 5 | 0.42 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 5 | 0.42 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 4 | 0.42 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 4 | 0.42 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 4 | 0.42 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 4 | 0.42 |
| (1,1323) | 1:156:A:SER:HA | 1:162:A:THR:HA | 17 | 0.42 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 18 | 0.42 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 18 | 0.42 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 18 | 0.42 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 18 | 0.42 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 19 | 0.42 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG21 | 7 | 0.42 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG22 | 7 | 0.42 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG23 | 7 | 0.42 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 15 | 0.42 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 11 | 0.42 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 18 | 0.42 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 19 | 0.42 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 3 | 0.42 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 3 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 3 | 0.42 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 3 | 0.42 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 3 | 0.42 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 3 | 0.42 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 12 | 0.42 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 12 | 0.42 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 12 | 0.42 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 12 | 0.42 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 12 | 0.42 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 13 | 0.42 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 13 | 0.42 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 15 | 0.42 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 15 | 0.42 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 15 | 0.42 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 20 | 0.42 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 20 | 0.42 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 20 | 0.42 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 9 | 0.42 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 9 | 0.42 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 9 | 0.42 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 7 | 0.42 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 2 | 0.42 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 19 | 0.42 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 19 | 0.42 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 19 | 0.42 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 19 | 0.42 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 19 | 0.42 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 19 | 0.42 |
| (1,893) | 1:155:A:LYS:HE3 | 1:166:A:ASP:H | 9 | 0.42 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 12 | 0.42 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 4 | 0.42 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 4 | 0.42 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 4 | 0.42 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 17 | 0.42 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 17 | 0.42 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 17 | 0.42 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 17 | 0.42 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 17 | 0.42 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 17 | 0.42 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 1 | 0.42 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 1 | 0.42 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 1 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,812) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG13 | 12 | 0.42 |
| (1,812) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG13 | 12 | 0.42 |
| (1,812) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG13 | 12 | 0.42 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 7 | 0.42 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 3 | 0.42 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 3 | 0.42 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 3 | 0.42 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 12 | 0.42 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 12 | 0.42 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 12 | 0.42 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 12 | 0.42 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 12 | 0.42 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 13 | 0.42 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 13 | 0.42 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 13 | 0.42 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 13 | 0.42 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 13 | 0.42 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 13 | 0.42 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 20 | 0.42 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 20 | 0.42 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 20 | 0.42 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 10 | 0.42 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 6 | 0.42 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 11 | 0.42 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 11 | 0.42 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 11 | 0.42 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 2 | 0.42 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG2 | 1 | 0.42 |
| (1,426) | 1:54:A:ILE:HG13 | 1:76:A:MET:HG3 | 1 | 0.42 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 10 | 0.42 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 10 | 0.42 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 10 | 0.42 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 1 | 0.42 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 1 | 0.42 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 1 | 0.42 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 12 | 0.42 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 3 | 0.42 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 3 | 0.42 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 3 | 0.42 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 17 | 0.42 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 17 | 0.42 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 17 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,145) | 1:55:A:ASN:HB3 | 2:12:B:ASN:HA | 8 | 0.42 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 10 | 0.42 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 10 | 0.42 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 10 | 0.42 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 1 | 0.42 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 1 | 0.42 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 1 | 0.42 |
| (1,65) | 1:52:A:VAL:HG11 | 1:76:A:MET:H | 7 | 0.42 |
| (1,65) | 1:52:A:VAL:HG12 | 1:76:A:MET:H | 7 | 0.42 |
| (1,65) | 1:52:A:VAL:HG13 | 1:76:A:MET:H | 7 | 0.42 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 1 | 0.42 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 15 | 0.42 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 10 | 0.42 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 10 | 0.42 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 10 | 0.42 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD21 | 9 | 0.42 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD22 | 9 | 0.42 |
| (1,6) | 1:47:A:THR:HA | 1:50:A:LEU:HD23 | 9 | 0.42 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 10 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 10 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 10 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 10 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 10 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 10 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 14 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 14 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 14 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 14 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 14 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 14 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 19 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 19 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 19 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 19 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 19 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 19 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 20 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 20 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 20 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 20 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 20 | 0.41 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 20 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 20 | 0.41 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 20 | 0.41 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 20 | 0.41 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 20 | 0.41 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 20 | 0.41 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 20 | 0.41 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 20 | 0.41 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 20 | 0.41 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 2 | 0.41 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 2 | 0.41 |
| (1,3826) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 7 | 0.41 |
| (1,3826) | 1:123:A:LYS:H | 1:123:A:LYS:HE3 | 7 | 0.41 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 16 | 0.41 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 16 | 0.41 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 13 | 0.41 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 13 | 0.41 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 13 | 0.41 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 13 | 0.41 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 13 | 0.41 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 13 | 0.41 |
| (1,3672) | 1:91:A:GLN:HB2 | 1:92:A:LYS:H | 4 | 0.41 |
| (1,3672) | 1:91:A:GLN:HB3 | 1:92:A:LYS:H | 4 | 0.41 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 4 | 0.41 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 4 | 0.41 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 8 | 0.41 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 8 | 0.41 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 8 | 0.41 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 8 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 3 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 3 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 3 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 3 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 18 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 18 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 18 | 0.41 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 18 | 0.41 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 5 | 0.41 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 8 | 0.41 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 17 | 0.41 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 13 | 0.41 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 13 | 0.41 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 17 | 0.41 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 17 | 0.41 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 17 | 0.41 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 3 | 0.41 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 3 | 0.41 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 3 | 0.41 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 20 | 0.41 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 20 | 0.41 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 20 | 0.41 |
| (1,3417) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HG2 | 4 | 0.41 |
| (1,3417) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HG3 | 4 | 0.41 |
| (1,3417) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HG2 | 4 | 0.41 |
| (1,3417) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HG3 | 4 | 0.41 |
| (1,3417) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HG2 | 4 | 0.41 |
| (1,3417) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HG3 | 4 | 0.41 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD2 | 6 | 0.41 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD3 | 6 | 0.41 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 20 | 0.41 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 19 | 0.41 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 12 | 0.41 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 12 | 0.41 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 12 | 0.41 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 4 | 0.41 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 4 | 0.41 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 14 | 0.41 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 14 | 0.41 |
| (1,3096) | 1:60:A:LYS:HE3 | 1:61:A:GLY:H | 11 | 0.41 |
| (1,3074) | 1:167:A:ASP:H | 1:196:A:ASN:HD22 | 13 | 0.41 |
| (1,3045) | 1:197:A:ALA:H | 1:225:A:LYS:H | 4 | 0.41 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 3 | 0.41 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 3 | 0.41 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 19 | 0.41 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 19 | 0.41 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 19 | 0.41 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 9 | 0.41 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 11 | 0.41 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 11 | 0.41 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 20 | 0.41 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 6 | 0.41 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 10 | 0.41 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 18 | 0.41 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 19 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 16 | 0.41 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 17 | 0.41 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 20 | 0.41 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 7 | 0.41 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 7 | 0.41 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 7 | 0.41 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 17 | 0.41 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 17 | 0.41 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 17 | 0.41 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 3 | 0.41 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 3 | 0.41 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 19 | 0.41 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 19 | 0.41 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 14 | 0.41 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 12 | 0.41 |
| (1,2105) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD3 | 3 | 0.41 |
| (1,2105) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD3 | 3 | 0.41 |
| (1,2105) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD3 | 3 | 0.41 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 19 | 0.41 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 19 | 0.41 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 19 | 0.41 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 10 | 0.41 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 10 | 0.41 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 10 | 0.41 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 13 | 0.41 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 13 | 0.41 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 13 | 0.41 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 4 | 0.41 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 11 | 0.41 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 19 | 0.41 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 15 | 0.41 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 15 | 0.41 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 15 | 0.41 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 19 | 0.41 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 3 | 0.41 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 1 | 0.41 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 1 | 0.41 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 1 | 0.41 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD21 | 12 | 0.41 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD22 | 12 | 0.41 |
| (1,1504) | 1:181:A:GLU:HA | 1:216:A:LEU:HD23 | 12 | 0.41 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 19 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 6 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 6 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 6 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 6 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 6 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 6 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 20 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 20 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 20 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 20 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 20 | 0.41 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 20 | 0.41 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 12 | 0.41 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 13 | 0.41 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 14 | 0.41 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 7 | 0.41 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 7 | 0.41 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 7 | 0.41 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 7 | 0.41 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 2 | 0.41 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 2 | 0.41 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 2 | 0.41 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 14 | 0.41 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 14 | 0.41 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 14 | 0.41 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 6 | 0.41 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 3 | 0.41 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 3 | 0.41 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 3 | 0.41 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 8 | 0.41 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 8 | 0.41 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 8 | 0.41 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 8 | 0.41 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 15 | 0.41 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 18 | 0.41 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 18 | 0.41 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 2 | 0.41 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 2 | 0.41 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 4 | 0.41 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 4 | 0.41 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 9 | 0.41 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 9 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 16 | 0.41 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 16 | 0.41 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 16 | 0.41 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 18 | 0.41 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 18 | 0.41 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 18 | 0.41 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 19 | 0.41 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 19 | 0.41 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 19 | 0.41 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 13 | 0.41 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 13 | 0.41 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 13 | 0.41 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 2 | 0.41 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 2 | 0.41 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 2 | 0.41 |
| (1,1008) | 1:123:A:LYS:H | 1:136:A:TYR:HB3 | 7 | 0.41 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 4 | 0.41 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 10 | 0.41 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 15 | 0.41 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 15 | 0.41 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 15 | 0.41 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 15 | 0.41 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 15 | 0.41 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 15 | 0.41 |
| (1,664) | 1:103:A:THR:HA | 1:128:A:LEU:H | 5 | 0.41 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 7 | 0.41 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 7 | 0.41 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 19 | 0.41 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 19 | 0.41 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 5 | 0.41 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 5 | 0.41 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 5 | 0.41 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 6 | 0.41 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 6 | 0.41 |
| (1,414) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HA | 1 | 0.41 |
| (1,414) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HA | 1 | 0.41 |
| (1,414) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HA | 1 | 0.41 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 10 | 0.41 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 10 | 0.41 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 10 | 0.41 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 10 | 0.41 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 10 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 10 | 0.41 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 11 | 0.41 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 11 | 0.41 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 11 | 0.41 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 19 | 0.41 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 19 | 0.41 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 19 | 0.41 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 19 | 0.41 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 19 | 0.41 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 19 | 0.41 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 7 | 0.41 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 11 | 0.41 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 20 | 0.41 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 20 | 0.41 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 20 | 0.41 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 3 | 0.41 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 3 | 0.41 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 3 | 0.41 |
| (1,339) | 1:173:A:TYR:HA | 1:205:A:LYS:HB2 | 18 | 0.41 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 9 | 0.41 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 5 | 0.41 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 5 | 0.41 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 5 | 0.41 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 19 | 0.41 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 19 | 0.41 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 19 | 0.41 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 2 | 0.41 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 4 | 0.41 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 4 | 0.41 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 17 | 0.41 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 17 | 0.41 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 6 | 0.4 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 6 | 0.4 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 12 | 0.4 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 12 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 12 | 0.4 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 12 | 0.4 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 7 | 0.4 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 7 | 0.4 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 7 | 0.4 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 7 | 0.4 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 7 | 0.4 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 7 | 0.4 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 1 | 0.4 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 1 | 0.4 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 1 | 0.4 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 1 | 0.4 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 1 | 0.4 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 1 | 0.4 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 4 | 0.4 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 4 | 0.4 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 9 | 0.4 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 9 | 0.4 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 9 | 0.4 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 9 | 0.4 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 9 | 0.4 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 9 | 0.4 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 10 | 0.4 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 10 | 0.4 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 4 | 0.4 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 4 | 0.4 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 4 | 0.4 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 4 | 0.4 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 4 | 0.4 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 4 | 0.4 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 4 | 0.4 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 4 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 8 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 8 | 0.4 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 8 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 14 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 14 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 14 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 14 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 14 | 0.4 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 14 | 0.4 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 18 | 0.4 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 18 | 0.4 |
| (1,3547) | 1:52:A:VAL:HG11 | 1:77:A:GLN:HG2 | 10 | 0.4 |
| (1,3547) | 1:52:A:VAL:HG11 | 1:77:A:GLN:HG3 | 10 | 0.4 |
| (1,3547) | 1:52:A:VAL:HG12 | 1:77:A:GLN:HG2 | 10 | 0.4 |
| (1,3547) | 1:52:A:VAL:HG12 | 1:77:A:GLN:HG3 | 10 | 0.4 |
| (1,3547) | 1:52:A:VAL:HG13 | 1:77:A:GLN:HG2 | 10 | 0.4 |
| (1,3547) | 1:52:A:VAL:HG13 | 1:77:A:GLN:HG3 | 10 | 0.4 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 4 | 0.4 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 4 | 0.4 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 4 | 0.4 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 12 | 0.4 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 16 | 0.4 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 16 | 0.4 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 16 | 0.4 |
| (1,3474) | 2:17:B:LYS:HD2 | 2:18:B:CYS:H | 2 | 0.4 |
| (1,3474) | 2:17:B:LYS:HD3 | 2:18:B:CYS:H | 2 | 0.4 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 3 | 0.4 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 3 | 0.4 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 2 | 0.4 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 8 | 0.4 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 8 | 0.4 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 8 | 0.4 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 5 | 0.4 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 5 | 0.4 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 6 | 0.4 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 6 | 0.4 |
| (1,3172) | 1:140:A:ILE:HB | 1:165:A:PHE:HZ | 19 | 0.4 |
| (1,3126) | 1:112:A:TYR:HE1 | 1:114:A:ASP:H | 7 | 0.4 |
| (1,3126) | 1:112:A:TYR:HE2 | 1:114:A:ASP:H | 7 | 0.4 |
| (1,3117) | 1:63:A:TYR:HD1 | 2:21:B:MET:HE1 | 2 | 0.4 |
| (1,3117) | 1:63:A:TYR:HD1 | 2:21:B:MET:HE2 | 2 | 0.4 |
| (1,3117) | 1:63:A:TYR:HD1 | 2:21:B:MET:HE3 | 2 | 0.4 |
| (1,3117) | 1:63:A:TYR:HD2 | 2:21:B:MET:HE1 | 2 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3117) | 1:63:A:TYR:HD2 | 2:21:B:MET:HE2 | 2 | 0.4 |
| (1,3117) | 1:63:A:TYR:HD2 | 2:21:B:MET:HE3 | 2 | 0.4 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 12 | 0.4 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 7 | 0.4 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 14 | 0.4 |
| (1,3057) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 14 | 0.4 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 6 | 0.4 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 18 | 0.4 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 19 | 0.4 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 19 | 0.4 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 5 | 0.4 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 6 | 0.4 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 4 | 0.4 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 3 | 0.4 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 8 | 0.4 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 12 | 0.4 |
| (1,2809) | 1:174:A:GLU:HG2 | 1:175:A:ASN:H | 18 | 0.4 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 8 | 0.4 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 8 | 0.4 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 8 | 0.4 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 11 | 0.4 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 8 | 0.4 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 2 | 0.4 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 2 | 0.4 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 4 | 0.4 |
| (1,2375) | 1:92:A:LYS:HG2 | 1:93:A:GLU:H | 8 | 0.4 |
| (1,2375) | 1:92:A:LYS:HG3 | 1:93:A:GLU:H | 8 | 0.4 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 17 | 0.4 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 4 | 0.4 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 14 | 0.4 |
| (1,2127) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB2 | 1 | 0.4 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 20 | 0.4 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 5 | 0.4 |
| (1,2072) | 1:223:A:THR:HB | 1:224:A:LEU:HG | 15 | 0.4 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 7 | 0.4 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 7 | 0.4 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 7 | 0.4 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 7 | 0.4 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 7 | 0.4 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 7 | 0.4 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 8 | 0.4 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 8 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 8 | 0.4 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 16 | 0.4 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 18 | 0.4 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 18 | 0.4 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 18 | 0.4 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 18 | 0.4 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 13 | 0.4 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 13 | 0.4 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 11 | 0.4 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 4 | 0.4 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 13 | 0.4 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE2 | 9 | 0.4 |
| (1,1768) | 1:200:A:ALA:HA | 1:205:A:LYS:HE3 | 9 | 0.4 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 7 | 0.4 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 7 | 0.4 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 7 | 0.4 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 20 | 0.4 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 20 | 0.4 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 20 | 0.4 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 4 | 0.4 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 17 | 0.4 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 17 | 0.4 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 17 | 0.4 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 5 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 7 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 7 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 7 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 7 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 7 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 7 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 14 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 14 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 14 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 14 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 14 | 0.4 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 14 | 0.4 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 10 | 0.4 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 1 | 0.4 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 6 | 0.4 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 6 | 0.4 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 6 | 0.4 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB2 | 3 | 0.4 |
| (1,1339) | 1:155:A:LYS:H | 1:163:A:LEU:HB3 | 3 | 0.4 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 5 | 0.4 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 5 | 0.4 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 5 | 0.4 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 5 | 0.4 |
| (1,1321) | 1:158:A:ASP:HB2 | 1:162:A:THR:HA | 1 | 0.4 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 8 | 0.4 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 19 | 0.4 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 2 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 6 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 6 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 6 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 11 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 11 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 11 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 16 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 16 | 0.4 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 16 | 0.4 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 3 | 0.4 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 3 | 0.4 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 3 | 0.4 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 3 | 0.4 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 3 | 0.4 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 3 | 0.4 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 1 | 0.4 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 1 | 0.4 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 1 | 0.4 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 6 | 0.4 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 6 | 0.4 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 6 | 0.4 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 1 | 0.4 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 1 | 0.4 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 1 | 0.4 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 3 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 5 | 0.4 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG11 | 6 | 0.4 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG12 | 6 | 0.4 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG13 | 6 | 0.4 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 10 | 0.4 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 19 | 0.4 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 4 | 0.4 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 4 | 0.4 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 4 | 0.4 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 4 | 0.4 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 4 | 0.4 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 4 | 0.4 |
| (1,794) | 1:73:A:VAL:HG11 | 1:83:A:GLN:HG2 | 10 | 0.4 |
| (1,794) | 1:73:A:VAL:HG12 | 1:83:A:GLN:HG2 | 10 | 0.4 |
| (1,794) | 1:73:A:VAL:HG13 | 1:83:A:GLN:HG2 | 10 | 0.4 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 9 | 0.4 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 13 | 0.4 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 13 | 0.4 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB1 | 19 | 0.4 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB2 | 19 | 0.4 |
| (1,707) | 1:84:A:ALA:HA | 1:106:A:ALA:HB3 | 19 | 0.4 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 2 | 0.4 |
| (1,637) | 1:146:A:PRO:HG3 | 1:147:A:GLY:H | 19 | 0.4 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 7 | 0.4 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 7 | 0.4 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG11 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG12 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG13 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG21 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG22 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD11 | 1:87:A:VAL:HG23 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG11 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG12 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG13 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG21 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG22 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD12 | 1:87:A:VAL:HG23 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG11 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG12 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG13 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG21 | 4 | 0.4 |
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG22 | 4 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,525) | 1:54:A:ILE:HD13 | 1:87:A:VAL:HG23 | 4 | 0.4 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 18 | 0.4 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 18 | 0.4 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 8 | 0.4 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 8 | 0.4 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 1 | 0.4 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 1 | 0.4 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 1 | 0.4 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 14 | 0.4 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 14 | 0.4 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 14 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 4 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 4 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 4 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 15 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 15 | 0.4 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 15 | 0.4 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 11 | 0.4 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 11 | 0.4 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 11 | 0.4 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 15 | 0.4 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 15 | 0.4 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 15 | 0.4 |
| (1,183) | 1:58:A:HIS:HB3 | 2:12:B:ASN:HD22 | 5 | 0.4 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 10 | 0.4 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 10 | 0.4 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 10 | 0.4 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 1 | 0.4 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 8 | 0.39 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 8 | 0.39 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 10 | 0.39 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 10 | 0.39 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 10 | 0.39 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 10 | 0.39 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 10 | 0.39 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 10 | 0.39 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 7 | 0.39 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 7 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 7 | 0.39 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 7 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 9 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 9 | 0.39 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 9 | 0.39 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 6 | 0.39 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 6 | 0.39 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 6 | 0.39 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 6 | 0.39 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 11 | 0.39 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 11 | 0.39 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 11 | 0.39 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 11 | 0.39 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 11 | 0.39 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 11 | 0.39 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 13 | 0.39 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 13 | 0.39 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 13 | 0.39 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 13 | 0.39 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 1 | 0.39 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 1 | 0.39 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 1 | 0.39 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 1 | 0.39 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 1 | 0.39 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 1 | 0.39 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 10 | 0.39 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 10 | 0.39 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 10 | 0.39 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 10 | 0.39 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 10 | 0.39 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 10 | 0.39 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 14 | 0.39 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 19 | 0.39 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 16 | 0.39 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 16 | 0.39 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 16 | 0.39 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 16 | 0.39 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 16 | 0.39 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 16 | 0.39 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 16 | 0.39 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 16 | 0.39 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 16 | 0.39 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 15 | 0.39 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 15 | 0.39 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 15 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 7 | 0.39 |
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 7 | 0.39 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 7 | 0.39 |
| (1,3474) | 2:17:B:LYS:HD2 | 2:18:B:CYS:H | 7 | 0.39 |
| (1,3474) | 2:17:B:LYS:HD3 | 2:18:B:CYS:H | 7 | 0.39 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 13 | 0.39 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 13 | 0.39 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 7 | 0.39 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 7 | 0.39 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 6 | 0.39 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 15 | 0.39 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 15 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 1 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 1 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 1 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 6 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 6 | 0.39 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 6 | 0.39 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 7 | 0.39 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 7 | 0.39 |
| (1,3116) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HA | 5 | 0.39 |
| (1,3116) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HA | 5 | 0.39 |
| (1,3116) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HA | 6 | 0.39 |
| (1,3116) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HA | 6 | 0.39 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 2 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 10 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 10 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 10 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 14 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 14 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 14 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 17 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 17 | 0.39 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 17 | 0.39 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 5 | 0.39 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 5 | 0.39 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 2 | 0.39 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 2 | 0.39 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 2 | 0.39 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 4 | 0.39 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 7 | 0.39 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 1 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 1 | 0.39 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 2 | 0.39 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 9 | 0.39 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 9 | 0.39 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 9 | 0.39 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 5 | 0.39 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 5 | 0.39 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 5 | 0.39 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 9 | 0.39 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 9 | 0.39 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 9 | 0.39 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 9 | 0.39 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 9 | 0.39 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 9 | 0.39 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 16 | 0.39 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 6 | 0.39 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 6 | 0.39 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 6 | 0.39 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 10 | 0.39 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 10 | 0.39 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 10 | 0.39 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 12 | 0.39 |
| (1,2544) | 1:128:A:LEU:HD11 | 1:131:A:LYS:H | 1 | 0.39 |
| (1,2544) | 1:128:A:LEU:HD12 | 1:131:A:LYS:H | 1 | 0.39 |
| (1,2544) | 1:128:A:LEU:HD13 | 1:131:A:LYS:H | 1 | 0.39 |
| (1,2544) | 1:128:A:LEU:HD21 | 1:131:A:LYS:H | 1 | 0.39 |
| (1,2544) | 1:128:A:LEU:HD22 | 1:131:A:LYS:H | 1 | 0.39 |
| (1,2544) | 1:128:A:LEU:HD23 | 1:131:A:LYS:H | 1 | 0.39 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 9 | 0.39 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 9 | 0.39 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 13 | 0.39 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 16 | 0.39 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 9 | 0.39 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 15 | 0.39 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD11 | 7 | 0.39 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD12 | 7 | 0.39 |
| (1,2284) | 1:75:A:ILE:H | 1:75:A:ILE:HD13 | 7 | 0.39 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 17 | 0.39 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 10 | 0.39 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 18 | 0.39 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 12 | 0.39 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 17 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 9 | 0.39 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 9 | 0.39 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 9 | 0.39 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 9 | 0.39 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 9 | 0.39 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 9 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 17 | 0.39 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 17 | 0.39 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 9 | 0.39 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 5 | 0.39 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 5 | 0.39 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 5 | 0.39 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 2 | 0.39 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 2 | 0.39 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 10 | 0.39 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 1 | 0.39 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 10 | 0.39 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 10 | 0.39 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 10 | 0.39 |
| (1,1727) | 1:168:A:ALA:H | 1:196:A:ASN:HB3 | 5 | 0.39 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 11 | 0.39 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 11 | 0.39 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 11 | 0.39 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 12 | 0.39 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 12 | 0.39 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 12 | 0.39 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 1 | 0.39 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 1 | 0.39 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 1 | 0.39 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 2 | 0.39 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 2 | 0.39 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 2 | 0.39 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 10 | 0.39 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 10 | 0.39 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 10 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 13 | 0.39 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 13 | 0.39 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 13 | 0.39 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 2 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 1 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 1 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 1 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 1 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 1 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 1 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 10 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 10 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 10 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 10 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 10 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 10 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 17 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 17 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 17 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 17 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 17 | 0.39 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 17 | 0.39 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 6 | 0.39 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 20 | 0.39 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 16 | 0.39 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 13 | 0.39 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 13 | 0.39 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 13 | 0.39 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 13 | 0.39 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 4 | 0.39 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 5 | 0.39 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 5 | 0.39 |
| (1,1225) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HB | 3 | 0.39 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 1 | 0.39 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 20 | 0.39 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 20 | 0.39 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 14 | 0.39 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 14 | 0.39 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 14 | 0.39 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 14 | 0.39 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 14 | 0.39 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 9 | 0.39 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 9 | 0.39 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 10 | 0.39 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 10 | 0.39 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 9 | 0.39 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 9 | 0.39 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 9 | 0.39 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 1 | 0.39 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 1 | 0.39 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 17 | 0.39 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 17 | 0.39 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 17 | 0.39 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 17 | 0.39 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 17 | 0.39 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 17 | 0.39 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 8 | 0.39 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 8 | 0.39 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 8 | 0.39 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 4 | 0.39 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 9 | 0.39 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 3 | 0.39 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 11 | 0.39 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 17 | 0.39 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 17 | 0.39 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 7 | 0.39 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 6 | 0.39 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 6 | 0.39 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 6 | 0.39 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 8 | 0.39 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 8 | 0.39 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 8 | 0.39 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 19 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 12 | 0.39 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 12 | 0.39 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 12 | 0.39 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 13 | 0.39 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 13 | 0.39 |
| (1,609) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 14 | 0.39 |
| (1,609) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 14 | 0.39 |
| (1,609) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 14 | 0.39 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 18 | 0.39 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 12 | 0.39 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 12 | 0.39 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 12 | 0.39 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 14 | 0.39 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 11 | 0.39 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 11 | 0.39 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 11 | 0.39 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 11 | 0.39 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 11 | 0.39 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 16 | 0.39 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 16 | 0.39 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 16 | 0.39 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 15 | 0.39 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 15 | 0.39 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 15 | 0.39 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 20 | 0.39 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 20 | 0.39 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 20 | 0.39 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 2 | 0.39 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 2 | 0.39 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 2 | 0.39 |
| (1,346) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HG3 | 8 | 0.39 |
| (1,346) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HG3 | 8 | 0.39 |
| (1,346) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HG3 | 8 | 0.39 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 4 | 0.39 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 4 | 0.39 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 4 | 0.39 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 4 | 0.39 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 4 | 0.39 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 4 | 0.39 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 9 | 0.39 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 9 | 0.39 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 9 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 17 | 0.38 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 17 | 0.38 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 17 | 0.38 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 17 | 0.38 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 17 | 0.38 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 17 | 0.38 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 5 | 0.38 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 5 | 0.38 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG11 | 2 | 0.38 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG12 | 2 | 0.38 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG13 | 2 | 0.38 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG21 | 2 | 0.38 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG22 | 2 | 0.38 |
| (1,3931) | 1:188:A:GLY:H | 1:189:A:VAL:HG23 | 2 | 0.38 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 1 | 0.38 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 1 | 0.38 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 1 | 0.38 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 1 | 0.38 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 1 | 0.38 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 1 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 1 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 1 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 6 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 6 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 20 | 0.38 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 20 | 0.38 |
| (1,3834) | 1:127:A:ASN:HB2 | 1:131:A:LYS:H | 8 | 0.38 |
| (1,3834) | 1:127:A:ASN:HB3 | 1:131:A:LYS:H | 8 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 2 | 0.38 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 2 | 0.38 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 17 | 0.38 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 17 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 17 | 0.38 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 17 | 0.38 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 17 | 0.38 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 17 | 0.38 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 19 | 0.38 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 19 | 0.38 |
| (1,3546) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA2 | 15 | 0.38 |
| (1,3546) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA3 | 15 | 0.38 |
| (1,3546) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA2 | 15 | 0.38 |
| (1,3546) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA3 | 15 | 0.38 |
| (1,3546) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA2 | 15 | 0.38 |
| (1,3546) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA3 | 15 | 0.38 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB2 | 18 | 0.38 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB3 | 18 | 0.38 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB2 | 18 | 0.38 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB3 | 18 | 0.38 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB2 | 18 | 0.38 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB3 | 18 | 0.38 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 18 | 0.38 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 18 | 0.38 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 18 | 0.38 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 18 | 0.38 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 11 | 0.38 |
| (1,3496) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HA | 3 | 0.38 |
| (1,3496) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HA | 3 | 0.38 |
| (1,3496) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HA | 3 | 0.38 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 4 | 0.38 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 4 | 0.38 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 4 | 0.38 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 16 | 0.38 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 16 | 0.38 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 16 | 0.38 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 2 | 0.38 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 2 | 0.38 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 2 | 0.38 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 2 | 0.38 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 2 | 0.38 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 2 | 0.38 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 3 | 0.38 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 3 | 0.38 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 4 | 0.38 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 4 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 1 | 0.38 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 1 | 0.38 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 1 | 0.38 |
| (1,3396) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HA | 5 | 0.38 |
| (1,3396) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HA | 5 | 0.38 |
| (1,3396) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HA | 5 | 0.38 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 1 | 0.38 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 1 | 0.38 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 17 | 0.38 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 5 | 0.38 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 15 | 0.38 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 10 | 0.38 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD1 | 7 | 0.38 |
| (1,3105) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HD2 | 7 | 0.38 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 16 | 0.38 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 8 | 0.38 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 16 | 0.38 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 9 | 0.38 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 13 | 0.38 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 5 | 0.38 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 5 | 0.38 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 5 | 0.38 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 16 | 0.38 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 11 | 0.38 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 16 | 0.38 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 13 | 0.38 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 4 | 0.38 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 4 | 0.38 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 4 | 0.38 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 16 | 0.38 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 17 | 0.38 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 12 | 0.38 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 12 | 0.38 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 12 | 0.38 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 16 | 0.38 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 16 | 0.38 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 16 | 0.38 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 7 | 0.38 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 7 | 0.38 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 7 | 0.38 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 16 | 0.38 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 16 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 16 | 0.38 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 20 | 0.38 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 6 | 0.38 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 2 | 0.38 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 2 | 0.38 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 13 | 0.38 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 15 | 0.38 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 7 | 0.38 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 13 | 0.38 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 13 | 0.38 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 16 | 0.38 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 4 | 0.38 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 4 | 0.38 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 4 | 0.38 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 14 | 0.38 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 14 | 0.38 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 14 | 0.38 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 15 | 0.38 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 15 | 0.38 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 15 | 0.38 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 15 | 0.38 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 15 | 0.38 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 15 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 14 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 16 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 16 | 0.38 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 16 | 0.38 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD11 | 15 | 0.38 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD12 | 15 | 0.38 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD13 | 15 | 0.38 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 2 | 0.38 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 2 | 0.38 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 2 | 0.38 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 12 | 0.38 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 12 | 0.38 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 12 | 0.38 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 3 | 0.38 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 3 | 0.38 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 3 | 0.38 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 17 | 0.38 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 17 | 0.38 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 17 | 0.38 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD2 | 5 | 0.38 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD3 | 5 | 0.38 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD2 | 5 | 0.38 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD3 | 5 | 0.38 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD2 | 5 | 0.38 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD3 | 5 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 2 | 0.38 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 2 | 0.38 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 4 | 0.38 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 9 | 0.38 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 9 | 0.38 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 9 | 0.38 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 1 | 0.38 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 17 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 17 | 0.38 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 17 | 0.38 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 8 | 0.38 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 8 | 0.38 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 8 | 0.38 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 13 | 0.38 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 13 | 0.38 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 13 | 0.38 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 14 | 0.38 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 14 | 0.38 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 14 | 0.38 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 4 | 0.38 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 2 | 0.38 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 2 | 0.38 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 2 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD11 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD12 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD11 | 1:201:A:ILE:HD13 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD11 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD12 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD12 | 1:201:A:ILE:HD13 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD11 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD12 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD13 | 1:201:A:ILE:HD13 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD11 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD12 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD21 | 1:201:A:ILE:HD13 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD11 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD12 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD22 | 1:201:A:ILE:HD13 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD11 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD12 | 3 | 0.38 |
| (1,1482) | 1:179:A:LEU:HD23 | 1:201:A:ILE:HD13 | 3 | 0.38 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 6 | 0.38 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 6 | 0.38 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 6 | 0.38 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 6 | 0.38 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 6 | 0.38 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 6 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 2 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 2 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 2 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 2 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 2 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 4 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 4 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 4 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 4 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 4 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 4 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 8 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 8 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 8 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 8 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 8 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 8 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 11 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 11 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 11 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 11 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 11 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 11 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 12 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 12 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 12 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 12 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 12 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 12 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 16 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 16 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 16 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 16 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 16 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 16 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 19 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 19 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 19 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 19 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 19 | 0.38 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 19 | 0.38 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 13 | 0.38 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 13 | 0.38 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 4 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 14 | 0.38 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD11 | 9 | 0.38 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD12 | 9 | 0.38 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD13 | 9 | 0.38 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD21 | 9 | 0.38 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD22 | 9 | 0.38 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD23 | 9 | 0.38 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 2 | 0.38 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 2 | 0.38 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 9 | 0.38 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 9 | 0.38 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 9 | 0.38 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 9 | 0.38 |
| (1,1305) | 1:161:A:LYS:HD2 | 1:189:A:VAL:HA | 9 | 0.38 |
| (1,1305) | 1:161:A:LYS:HD3 | 1:189:A:VAL:HA | 9 | 0.38 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 17 | 0.38 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 17 | 0.38 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 17 | 0.38 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 11 | 0.38 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 11 | 0.38 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 11 | 0.38 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 20 | 0.38 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 20 | 0.38 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 20 | 0.38 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 7 | 0.38 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 7 | 0.38 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 7 | 0.38 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 8 | 0.38 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 11 | 0.38 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 11 | 0.38 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 11 | 0.38 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 8 | 0.38 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 8 | 0.38 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 8 | 0.38 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 13 | 0.38 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 13 | 0.38 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 13 | 0.38 |
| (1,1111) | 1:116:A:GLN:HA | 1:142:A:THR:HA | 5 | 0.38 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 8 | 0.38 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 14 | 0.38 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 15 | 0.38 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 11 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 15 | 0.38 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB1 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB2 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB3 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB1 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB2 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB3 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB1 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB2 | 10 | 0.38 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB3 | 10 | 0.38 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 20 | 0.38 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 20 | 0.38 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 20 | 0.38 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG21 | 16 | 0.38 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG22 | 16 | 0.38 |
| (1,775) | 1:113:A:ASP:HA | 1:143:A:VAL:HG23 | 16 | 0.38 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 6 | 0.38 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 6 | 0.38 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 4 | 0.38 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 4 | 0.38 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 5 | 0.38 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 5 | 0.38 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 5 | 0.38 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 3 | 0.38 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 3 | 0.38 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 3 | 0.38 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 17 | 0.38 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 17 | 0.38 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 17 | 0.38 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 3 | 0.38 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 3 | 0.38 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 3 | 0.38 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 5 | 0.38 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 5 | 0.38 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 5 | 0.38 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 20 | 0.38 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 18 | 0.38 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 19 | 0.38 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 19 | 0.38 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 14 | 0.38 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 14 | 0.38 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 18 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 18 | 0.38 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 18 | 0.38 |
| (1,330) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HA | 15 | 0.38 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 8 | 0.38 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB1 | 6 | 0.38 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB2 | 6 | 0.38 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB3 | 6 | 0.38 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 9 | 0.38 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 9 | 0.38 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 9 | 0.38 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 9 | 0.38 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 14 | 0.38 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 14 | 0.38 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 14 | 0.38 |
| (1,81) | 1:52:A:VAL:HG11 | 1:53:A:THR:HB | 12 | 0.38 |
| (1,81) | 1:52:A:VAL:HG12 | 1:53:A:THR:HB | 12 | 0.38 |
| (1,81) | 1:52:A:VAL:HG13 | 1:53:A:THR:HB | 12 | 0.38 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 9 | 0.38 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 9 | 0.38 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 9 | 0.38 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 18 | 0.38 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 13 | 0.38 |
| (1,37) | 1:51:A:PRO:HA | 2:7:B:PRO:HD2 | 8 | 0.38 |
| (1,4046) | 2:19:B:GLN:HG2 | 2:21:B:MET:H | 11 | 0.37 |
| (1,4046) | 2:19:B:GLN:HG3 | 2:21:B:MET:H | 11 | 0.37 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 15 | 0.37 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 15 | 0.37 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 11 | 0.37 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 11 | 0.37 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 9 | 0.37 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 9 | 0.37 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 9 | 0.37 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 9 | 0.37 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 9 | 0.37 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 9 | 0.37 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 12 | 0.37 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 12 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 15 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 15 | 0.37 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 15 | 0.37 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 4 | 0.37 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 4 | 0.37 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 4 | 0.37 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 4 | 0.37 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 4 | 0.37 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 4 | 0.37 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 18 | 0.37 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 18 | 0.37 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 18 | 0.37 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 18 | 0.37 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 18 | 0.37 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 18 | 0.37 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 4 | 0.37 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 4 | 0.37 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 16 | 0.37 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 16 | 0.37 |
| (1,3768) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG13 | 14 | 0.37 |
| (1,3768) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 14 | 0.37 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 12 | 0.37 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 12 | 0.37 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 12 | 0.37 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 12 | 0.37 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 12 | 0.37 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 12 | 0.37 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 8 | 0.37 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 8 | 0.37 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 8 | 0.37 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 8 | 0.37 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 8 | 0.37 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 8 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 11 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 11 | 0.37 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 11 | 0.37 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 12 | 0.37 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 12 | 0.37 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD21 | 9 | 0.37 |
| (1,3536) | 1:47:A:THR:HG21 | 1:48:A:ASN:HD22 | 9 | 0.37 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD21 | 9 | 0.37 |
| (1,3536) | 1:47:A:THR:HG22 | 1:48:A:ASN:HD22 | 9 | 0.37 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD21 | 9 | 0.37 |
| (1,3536) | 1:47:A:THR:HG23 | 1:48:A:ASN:HD22 | 9 | 0.37 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 3 | 0.37 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 3 | 0.37 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 3 | 0.37 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 3 | 0.37 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 14 | 0.37 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 14 | 0.37 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 14 | 0.37 |
| (1,3521) | 1:59:A:ALA:HB1 | 2:12:B:ASN:HB2 | 4 | 0.37 |
| (1,3521) | 1:59:A:ALA:HB2 | 2:12:B:ASN:HB2 | 4 | 0.37 |
| (1,3521) | 1:59:A:ALA:HB3 | 2:12:B:ASN:HB2 | 4 | 0.37 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 2 | 0.37 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 2 | 0.37 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 13 | 0.37 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 13 | 0.37 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 11 | 0.37 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 11 | 0.37 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 11 | 0.37 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 19 | 0.37 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 19 | 0.37 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 19 | 0.37 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 2 | 0.37 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 2 | 0.37 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 2 | 0.37 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 18 | 0.37 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 18 | 0.37 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 18 | 0.37 |
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 19 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 19 | 0.37 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 19 | 0.37 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 14 | 0.37 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 14 | 0.37 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 14 | 0.37 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 14 | 0.37 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 14 | 0.37 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 14 | 0.37 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 20 | 0.37 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 20 | 0.37 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 20 | 0.37 |
| (1,3401) | 2:6:B:VAL:HG21 | 2:7:B:PRO:HD3 | 10 | 0.37 |
| (1,3401) | 2:6:B:VAL:HG22 | 2:7:B:PRO:HD3 | 10 | 0.37 |
| (1,3401) | 2:6:B:VAL:HG23 | 2:7:B:PRO:HD3 | 10 | 0.37 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD2 | 7 | 0.37 |
| (1,3382) | 2:17:B:LYS:H | 2:17:B:LYS:HD3 | 7 | 0.37 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 4 | 0.37 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 4 | 0.37 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB1 | 13 | 0.37 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB2 | 13 | 0.37 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB3 | 13 | 0.37 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 10 | 0.37 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 10 | 0.37 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 18 | 0.37 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 13 | 0.37 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 13 | 0.37 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 13 | 0.37 |
| (1,3050) | 1:225:A:LYS:H | 1:225:A:LYS:HB3 | 2 | 0.37 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 9 | 0.37 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 20 | 0.37 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 20 | 0.37 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 20 | 0.37 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 6 | 0.37 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 6 | 0.37 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 6 | 0.37 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 4 | 0.37 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 4 | 0.37 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 4 | 0.37 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 12 | 0.37 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 12 | 0.37 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 12 | 0.37 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 1 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB1 | 19 | 0.37 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB2 | 19 | 0.37 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB3 | 19 | 0.37 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 3 | 0.37 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 3 | 0.37 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 3 | 0.37 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 7 | 0.37 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 7 | 0.37 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 7 | 0.37 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 20 | 0.37 |
| (1,2761) | 1:167:A:ASP:H | 1:196:A:ASN:HB2 | 19 | 0.37 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 3 | 0.37 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 3 | 0.37 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 3 | 0.37 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 6 | 0.37 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 20 | 0.37 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 20 | 0.37 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 20 | 0.37 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 12 | 0.37 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 20 | 0.37 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 20 | 0.37 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 20 | 0.37 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 13 | 0.37 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 18 | 0.37 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 19 | 0.37 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 19 | 0.37 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 16 | 0.37 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 5 | 0.37 |
| (1,2407) | 1:88:A:GLN:H | 1:107:A:LEU:HB2 | 2 | 0.37 |
| (1,2407) | 1:88:A:GLN:H | 1:107:A:LEU:HB3 | 2 | 0.37 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 9 | 0.37 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 16 | 0.37 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 9 | 0.37 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 3 | 0.37 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 3 | 0.37 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 3 | 0.37 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 2 | 0.37 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 7 | 0.37 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD11 | 12 | 0.37 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD12 | 12 | 0.37 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD13 | 12 | 0.37 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 14 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 14 | 0.37 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 14 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 4 | 0.37 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 4 | 0.37 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 10 | 0.37 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 10 | 0.37 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 10 | 0.37 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 5 | 0.37 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 5 | 0.37 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 19 | 0.37 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 19 | 0.37 |
| (1,1870) | 1:202:A:THR:H | 1:205:A:LYS:HD2 | 11 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 5 | 0.37 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 5 | 0.37 |
| (1,1731) | 1:167:A:ASP:HA | 1:196:A:ASN:HB3 | 5 | 0.37 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 13 | 0.37 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 13 | 0.37 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 13 | 0.37 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 14 | 0.37 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 14 | 0.37 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 14 | 0.37 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 9 | 0.37 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 9 | 0.37 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 9 | 0.37 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 14 | 0.37 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 16 | 0.37 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 16 | 0.37 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 5 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 5 | 0.37 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 5 | 0.37 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 19 | 0.37 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 19 | 0.37 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 19 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 5 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 5 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 5 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 5 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 5 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 5 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 13 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 13 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 13 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 13 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 13 | 0.37 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 13 | 0.37 |
| (1,1321) | 1:158:A:ASP:HB2 | 1:162:A:THR:HA | 5 | 0.37 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 5 | 0.37 |
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 11 | 0.37 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 11 | 0.37 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 11 | 0.37 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 14 | 0.37 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 14 | 0.37 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 14 | 0.37 |
| (1,1205) | 1:151:A:ALA:HA | 1:152:A:LYS:HG3 | 10 | 0.37 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 16 | 0.37 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 19 | 0.37 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 19 | 0.37 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 19 | 0.37 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 19 | 0.37 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 19 | 0.37 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 19 | 0.37 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 1 | 0.37 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 1 | 0.37 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 1 | 0.37 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 19 | 0.37 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 19 | 0.37 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 2 | 0.37 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 2 | 0.37 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 2 | 0.37 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 8 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 8 | 0.37 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 8 | 0.37 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 8 | 0.37 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 8 | 0.37 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 8 | 0.37 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 7 | 0.37 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 7 | 0.37 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 7 | 0.37 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 7 | 0.37 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 7 | 0.37 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 7 | 0.37 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 2 | 0.37 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 2 | 0.37 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 13 | 0.37 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 13 | 0.37 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 9 | 0.37 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 9 | 0.37 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 9 | 0.37 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 13 | 0.37 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 13 | 0.37 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 13 | 0.37 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 13 | 0.37 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 13 | 0.37 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 13 | 0.37 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 13 | 0.37 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 13 | 0.37 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 13 | 0.37 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 19 | 0.37 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 9 | 0.37 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 8 | 0.37 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 17 | 0.37 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 17 | 0.37 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 17 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 4 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 4 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 4 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 9 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 9 | 0.37 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 9 | 0.37 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 8 | 0.37 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 18 | 0.37 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 18 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 18 | 0.37 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 18 | 0.37 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 18 | 0.37 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 18 | 0.37 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 15 | 0.37 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 15 | 0.37 |
| (1,605) | 1:81:A:ARG:H | 1:114:A:ASP:HA | 5 | 0.37 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 1 | 0.37 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 19 | 0.37 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 19 | 0.37 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 19 | 0.37 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 17 | 0.37 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 17 | 0.37 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 5 | 0.37 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 5 | 0.37 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 3 | 0.37 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 12 | 0.37 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 12 | 0.37 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 12 | 0.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 3 | 0.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 3 | 0.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 3 | 0.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD11 | 18 | 0.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD12 | 18 | 0.37 |
| (1,392) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HD13 | 18 | 0.37 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 2 | 0.37 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 2 | 0.37 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 2 | 0.37 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 2 | 0.37 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 20 | 0.37 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 9 | 0.37 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 9 | 0.37 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 9 | 0.37 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 6 | 0.37 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 6 | 0.37 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 6 | 0.37 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 16 | 0.37 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 16 | 0.37 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 16 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 1 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 1 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 1 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 8 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 8 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 8 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 16 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 16 | 0.37 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 16 | 0.37 |
| (1,65) | 1:52:A:VAL:HG11 | 1:76:A:MET:H | 18 | 0.37 |
| (1,65) | 1:52:A:VAL:HG12 | 1:76:A:MET:H | 18 | 0.37 |
| (1,65) | 1:52:A:VAL:HG13 | 1:76:A:MET:H | 18 | 0.37 |
| (1,50) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD2 | 16 | 0.37 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 12 | 0.37 |
| (1,37) | 1:51:A:PRO:HA | 2:7:B:PRO:HD2 | 4 | 0.37 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 8 | 0.36 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 8 | 0.36 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 8 | 0.36 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 8 | 0.36 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 8 | 0.36 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 8 | 0.36 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 13 | 0.36 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 13 | 0.36 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 5 | 0.36 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 5 | 0.36 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 9 | 0.36 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 9 | 0.36 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD11 | 3 | 0.36 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD12 | 3 | 0.36 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD13 | 3 | 0.36 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD21 | 3 | 0.36 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD22 | 3 | 0.36 |
| (1,3909) | 1:180:A:ILE:HA | 1:220:A:LEU:HD23 | 3 | 0.36 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 11 | 0.36 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 11 | 0.36 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 13 | 0.36 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 13 | 0.36 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 3 | 0.36 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 3 | 0.36 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 6 | 0.36 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB3 | 6 | 0.36 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 1 | 0.36 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 1 | 0.36 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 11 | 0.36 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 14 | 0.36 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 14 | 0.36 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 16 | 0.36 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 16 | 0.36 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 1 | 0.36 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 1 | 0.36 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 8 | 0.36 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 8 | 0.36 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 1 | 0.36 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 1 | 0.36 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG21 | 16 | 0.36 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG22 | 16 | 0.36 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG23 | 16 | 0.36 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG21 | 16 | 0.36 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG22 | 16 | 0.36 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG23 | 16 | 0.36 |
| (1,3538) | 1:48:A:ASN:HD21 | 1:49:A:ASP:H | 11 | 0.36 |
| (1,3538) | 1:48:A:ASN:HD22 | 1:49:A:ASP:H | 11 | 0.36 |
| (1,3520) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HG12 | 7 | 0.36 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG21 | 17 | 0.36 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG22 | 17 | 0.36 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG23 | 17 | 0.36 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG21 | 17 | 0.36 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG22 | 17 | 0.36 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG23 | 17 | 0.36 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 1 | 0.36 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 2 | 0.36 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 3 | 0.36 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 3 | 0.36 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 3 | 0.36 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 3 | 0.36 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 3 | 0.36 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 3 | 0.36 |
| (1,3479) | 1:53:A:THR:HG21 | 2:9:B:ILE:HB | 13 | 0.36 |
| (1,3479) | 1:53:A:THR:HG22 | 2:9:B:ILE:HB | 13 | 0.36 |
| (1,3479) | 1:53:A:THR:HG23 | 2:9:B:ILE:HB | 13 | 0.36 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 10 | 0.36 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 10 | 0.36 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 10 | 0.36 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 10 | 0.36 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 10 | 0.36 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 10 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 16 | 0.36 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 16 | 0.36 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 16 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 5 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 5 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 5 | 0.36 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 5 | 0.36 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 1 | 0.36 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 13 | 0.36 |
| (1,3282) | 1:69:A:PHE:HZ | 2:8:B:ILE:HD11 | 12 | 0.36 |
| (1,3282) | 1:69:A:PHE:HZ | 2:8:B:ILE:HD12 | 12 | 0.36 |
| (1,3282) | 1:69:A:PHE:HZ | 2:8:B:ILE:HD13 | 12 | 0.36 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 10 | 0.36 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 12 | 0.36 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 12 | 0.36 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 10 | 0.36 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 16 | 0.36 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 16 | 0.36 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 16 | 0.36 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 4 | 0.36 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 6 | 0.36 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 6 | 0.36 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 6 | 0.36 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 3 | 0.36 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 3 | 0.36 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 3 | 0.36 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 7 | 0.36 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 7 | 0.36 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 7 | 0.36 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 12 | 0.36 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 12 | 0.36 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 20 | 0.36 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 20 | 0.36 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 18 | 0.36 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 18 | 0.36 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 18 | 0.36 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 13 | 0.36 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 14 | 0.36 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 19 | 0.36 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 17 | 0.36 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 8 | 0.36 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 11 | 0.36 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 11 | 0.36 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 17 | 0.36 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 17 | 0.36 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 17 | 0.36 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 8 | 0.36 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 15 | 0.36 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 15 | 0.36 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 15 | 0.36 |
| (1,2565) | 1:137:A:ASP:H | 1:154:A:ILE:HG13 | 14 | 0.36 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 1 | 0.36 |
| (1,2544) | 1:128:A:LEU:HD11 | 1:131:A:LYS:H | 19 | 0.36 |
| (1,2544) | 1:128:A:LEU:HD12 | 1:131:A:LYS:H | 19 | 0.36 |
| (1,2544) | 1:128:A:LEU:HD13 | 1:131:A:LYS:H | 19 | 0.36 |
| (1,2544) | 1:128:A:LEU:HD21 | 1:131:A:LYS:H | 19 | 0.36 |
| (1,2544) | 1:128:A:LEU:HD22 | 1:131:A:LYS:H | 19 | 0.36 |
| (1,2544) | 1:128:A:LEU:HD23 | 1:131:A:LYS:H | 19 | 0.36 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 15 | 0.36 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 15 | 0.36 |
| (1,2375) | 1:92:A:LYS:HG2 | 1:93:A:GLU:H | 16 | 0.36 |
| (1,2375) | 1:92:A:LYS:HG3 | 1:93:A:GLU:H | 16 | 0.36 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 18 | 0.36 |
| (1,2228) | 1:65:A:ASP:H | 1:67:A:ALA:HB1 | 6 | 0.36 |
| (1,2228) | 1:65:A:ASP:H | 1:67:A:ALA:HB2 | 6 | 0.36 |
| (1,2228) | 1:65:A:ASP:H | 1:67:A:ALA:HB3 | 6 | 0.36 |
| (1,2127) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB2 | 11 | 0.36 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 8 | 0.36 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 8 | 0.36 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 3 | 0.36 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 11 | 0.36 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 11 | 0.36 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 11 | 0.36 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 16 | 0.36 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 2 | 0.36 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 2 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 2 | 0.36 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 14 | 0.36 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 14 | 0.36 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 14 | 0.36 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 18 | 0.36 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 18 | 0.36 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 5 | 0.36 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 5 | 0.36 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 5 | 0.36 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 5 | 0.36 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG21 | 7 | 0.36 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG22 | 7 | 0.36 |
| (1,1669) | 1:165:A:PHE:HB3 | 1:192:A:ILE:HG23 | 7 | 0.36 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 5 | 0.36 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 5 | 0.36 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 5 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 11 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 11 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 11 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 13 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 13 | 0.36 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 13 | 0.36 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 18 | 0.36 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 18 | 0.36 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 18 | 0.36 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 11 | 0.36 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 11 | 0.36 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 11 | 0.36 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 11 | 0.36 |
| (1,1591) | 1:181:A:GLU:H | 1:185:A:LYS:HE3 | 20 | 0.36 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 2 | 0.36 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 9 | 0.36 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 9 | 0.36 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 9 | 0.36 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 4 | 0.36 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 16 | 0.36 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 20 | 0.36 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 20 | 0.36 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 20 | 0.36 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 20 | 0.36 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 10 | 0.36 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1285) | 1:157:A:LEU:HD11 | 1:158:A:ASP:HA | 20 | 0.36 |
| (1,1285) | 1:157:A:LEU:HD12 | 1:158:A:ASP:HA | 20 | 0.36 |
| (1,1285) | 1:157:A:LEU:HD13 | 1:158:A:ASP:HA | 20 | 0.36 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 16 | 0.36 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 16 | 0.36 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 16 | 0.36 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 18 | 0.36 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 18 | 0.36 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 18 | 0.36 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 6 | 0.36 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 6 | 0.36 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 6 | 0.36 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 14 | 0.36 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 14 | 0.36 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 14 | 0.36 |
| (1,1120) | 1:142:A:THR:HG21 | 1:179:A:LEU:H | 12 | 0.36 |
| (1,1120) | 1:142:A:THR:HG22 | 1:179:A:LEU:H | 12 | 0.36 |
| (1,1120) | 1:142:A:THR:HG23 | 1:179:A:LEU:H | 12 | 0.36 |
| (1,1111) | 1:116:A:GLN:HA | 1:142:A:THR:HA | 18 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 18 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 18 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 18 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 18 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 18 | 0.36 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 18 | 0.36 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 11 | 0.36 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 11 | 0.36 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 20 | 0.36 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 20 | 0.36 |
| (1,1094) | 1:140:A:ILE:HG21 | 1:148:A:SER:H | 19 | 0.36 |
| (1,1094) | 1:140:A:ILE:HG22 | 1:148:A:SER:H | 19 | 0.36 |
| (1,1094) | 1:140:A:ILE:HG23 | 1:148:A:SER:H | 19 | 0.36 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 8 | 0.36 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 8 | 0.36 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 8 | 0.36 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 8 | 0.36 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 8 | 0.36 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 8 | 0.36 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 11 | 0.36 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 11 | 0.36 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 11 | 0.36 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 13 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 13 | 0.36 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 13 | 0.36 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 7 | 0.36 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 7 | 0.36 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 7 | 0.36 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 15 | 0.36 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 15 | 0.36 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 15 | 0.36 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 3 | 0.36 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 16 | 0.36 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 7 | 0.36 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 7 | 0.36 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 19 | 0.36 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 6 | 0.36 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 20 | 0.36 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 13 | 0.36 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 18 | 0.36 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 18 | 0.36 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 19 | 0.36 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 20 | 0.36 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 17 | 0.36 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 6 | 0.36 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 6 | 0.36 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 6 | 0.36 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 16 | 0.36 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 16 | 0.36 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 4 | 0.36 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 4 | 0.36 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 4 | 0.36 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 1 | 0.36 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 1 | 0.36 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 1 | 0.36 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 9 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 9 | 0.36 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 9 | 0.36 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 17 | 0.36 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 17 | 0.36 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 17 | 0.36 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 1 | 0.36 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 18 | 0.36 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 19 | 0.36 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 19 | 0.36 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 19 | 0.36 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 6 | 0.36 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 6 | 0.36 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 6 | 0.36 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 15 | 0.36 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 15 | 0.36 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 15 | 0.36 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 15 | 0.36 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 1 | 0.36 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 11 | 0.36 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 11 | 0.36 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 11 | 0.36 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG2 | 1 | 0.36 |
| (1,126) | 1:54:A:ILE:HG21 | 1:76:A:MET:HG3 | 1 | 0.36 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG2 | 1 | 0.36 |
| (1,126) | 1:54:A:ILE:HG22 | 1:76:A:MET:HG3 | 1 | 0.36 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG2 | 1 | 0.36 |
| (1,126) | 1:54:A:ILE:HG23 | 1:76:A:MET:HG3 | 1 | 0.36 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 3 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 5 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 5 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 5 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 10 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 10 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 10 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 11 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 11 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 11 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 18 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 18 | 0.36 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 18 | 0.36 |
| (1,12) | 1:47:A:THR:HB | 1:50:A:LEU:HG | 3 | 0.36 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 6 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 6 | 0.35 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 14 | 0.35 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 14 | 0.35 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 1 | 0.35 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 1 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 8 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 8 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 8 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 8 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 8 | 0.35 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 8 | 0.35 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 12 | 0.35 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 12 | 0.35 |
| (1,3672) | 1:91:A:GLN:HB2 | 1:92:A:LYS:H | 15 | 0.35 |
| (1,3672) | 1:91:A:GLN:HB3 | 1:92:A:LYS:H | 15 | 0.35 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 13 | 0.35 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 13 | 0.35 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 13 | 0.35 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 13 | 0.35 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 18 | 0.35 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 18 | 0.35 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 18 | 0.35 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 18 | 0.35 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 19 | 0.35 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 19 | 0.35 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 19 | 0.35 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 19 | 0.35 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 19 | 0.35 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 19 | 0.35 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 8 | 0.35 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 8 | 0.35 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 8 | 0.35 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 8 | 0.35 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 8 | 0.35 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 8 | 0.35 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 9 | 0.35 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 9 | 0.35 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 17 | 0.35 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 15 | 0.35 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 15 | 0.35 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 13 | 0.35 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 13 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 13 | 0.35 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 13 | 0.35 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 13 | 0.35 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 13 | 0.35 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 19 | 0.35 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 19 | 0.35 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 19 | 0.35 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG21 | 17 | 0.35 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG22 | 17 | 0.35 |
| (1,3438) | 2:12:B:ASN:HD21 | 2:15:B:THR:HG23 | 17 | 0.35 |
| (1,3420) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HG2 | 4 | 0.35 |
| (1,3420) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HG3 | 4 | 0.35 |
| (1,3420) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HG2 | 4 | 0.35 |
| (1,3420) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HG3 | 4 | 0.35 |
| (1,3420) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HG2 | 4 | 0.35 |
| (1,3420) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HG3 | 4 | 0.35 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 3 | 0.35 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 3 | 0.35 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 3 | 0.35 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 13 | 0.35 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 17 | 0.35 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 12 | 0.35 |
| (1,3239) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HA | 13 | 0.35 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 9 | 0.35 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 18 | 0.35 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 18 | 0.35 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 18 | 0.35 |
| (1,3223) | 1:103:A:THR:HB | 1:125:A:TRP:HD1 | 16 | 0.35 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 1 | 0.35 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 1 | 0.35 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 12 | 0.35 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 8 | 0.35 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 8 | 0.35 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 8 | 0.35 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 9 | 0.35 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 12 | 0.35 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 4 | 0.35 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 4 | 0.35 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 4 | 0.35 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 13 | 0.35 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 13 | 0.35 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 13 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 3 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 3 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 10 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 10 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 15 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 15 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 19 | 0.35 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 19 | 0.35 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 17 | 0.35 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 17 | 0.35 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 17 | 0.35 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 3 | 0.35 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 8 | 0.35 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 15 | 0.35 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 6 | 0.35 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 12 | 0.35 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 15 | 0.35 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 19 | 0.35 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 18 | 0.35 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 19 | 0.35 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 12 | 0.35 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 14 | 0.35 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 8 | 0.35 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 8 | 0.35 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 8 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 6 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 6 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 6 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 11 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 11 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 11 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 16 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 16 | 0.35 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 16 | 0.35 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 11 | 0.35 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 11 | 0.35 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 11 | 0.35 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 1 | 0.35 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 3 | 0.35 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 3 | 0.35 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 20 | 0.35 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 11 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 11 | 0.35 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 11 | 0.35 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 15 | 0.35 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 15 | 0.35 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 15 | 0.35 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 18 | 0.35 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 20 | 0.35 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 1 | 0.35 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 8 | 0.35 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 18 | 0.35 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 19 | 0.35 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 1 | 0.35 |
| (1,2202) | 1:59:A:ALA:H | 1:70:A:THR:HG21 | 20 | 0.35 |
| (1,2202) | 1:59:A:ALA:H | 1:70:A:THR:HG22 | 20 | 0.35 |
| (1,2202) | 1:59:A:ALA:H | 1:70:A:THR:HG23 | 20 | 0.35 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 13 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD11 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD12 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD13 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD11 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD12 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD13 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD11 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD12 | 3 | 0.35 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD13 | 3 | 0.35 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 11 | 0.35 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 11 | 0.35 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 11 | 0.35 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 17 | 0.35 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 17 | 0.35 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 10 | 0.35 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 20 | 0.35 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 20 | 0.35 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 20 | 0.35 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 20 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 20 | 0.35 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 20 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 7 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 7 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 7 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 16 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 16 | 0.35 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 16 | 0.35 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD11 | 12 | 0.35 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD12 | 12 | 0.35 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD13 | 12 | 0.35 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 2 | 0.35 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 14 | 0.35 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 4 | 0.35 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 4 | 0.35 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 4 | 0.35 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 7 | 0.35 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 7 | 0.35 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 7 | 0.35 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 16 | 0.35 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 16 | 0.35 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 16 | 0.35 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 19 | 0.35 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 4 | 0.35 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 11 | 0.35 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 14 | 0.35 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 14 | 0.35 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 14 | 0.35 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 14 | 0.35 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 13 | 0.35 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 13 | 0.35 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 13 | 0.35 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 17 | 0.35 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 1 | 0.35 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 19 | 0.35 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 14 | 0.35 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 14 | 0.35 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 14 | 0.35 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 16 | 0.35 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 16 | 0.35 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 16 | 0.35 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 16 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 16 | 0.35 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 16 | 0.35 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 7 | 0.35 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 17 | 0.35 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 8 | 0.35 |
| (1,1284) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 12 | 0.35 |
| (1,1284) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 12 | 0.35 |
| (1,1284) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 12 | 0.35 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 1 | 0.35 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 1 | 0.35 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 1 | 0.35 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 2 | 0.35 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 2 | 0.35 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 2 | 0.35 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 8 | 0.35 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 8 | 0.35 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 8 | 0.35 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 8 | 0.35 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 8 | 0.35 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 8 | 0.35 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 14 | 0.35 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 14 | 0.35 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 3 | 0.35 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 3 | 0.35 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 3 | 0.35 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 1 | 0.35 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 1 | 0.35 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 1 | 0.35 |
| (1,1125) | 1:118:A:ILE:HD11 | 1:143:A:VAL:HA | 10 | 0.35 |
| (1,1125) | 1:118:A:ILE:HD12 | 1:143:A:VAL:HA | 10 | 0.35 |
| (1,1125) | 1:118:A:ILE:HD13 | 1:143:A:VAL:HA | 10 | 0.35 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 4 | 0.35 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 4 | 0.35 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 19 | 0.35 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 14 | 0.35 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 16 | 0.35 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 12 | 0.35 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 17 | 0.35 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 17 | 0.35 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 17 | 0.35 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 17 | 0.35 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 17 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 17 | 0.35 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 6 | 0.35 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 5 | 0.35 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 9 | 0.35 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 9 | 0.35 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 9 | 0.35 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 6 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 7 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 7 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 7 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 19 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 19 | 0.35 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 19 | 0.35 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 10 | 0.35 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 10 | 0.35 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 15 | 0.35 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 15 | 0.35 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 16 | 0.35 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 16 | 0.35 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 6 | 0.35 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 18 | 0.35 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB2 | 1 | 0.35 |
| (1,739) | 1:158:A:ASP:HB2 | 1:161:A:LYS:HB3 | 1 | 0.35 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 13 | 0.35 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 13 | 0.35 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 13 | 0.35 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 13 | 0.35 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 13 | 0.35 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 13 | 0.35 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 4 | 0.35 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 16 | 0.35 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 16 | 0.35 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 16 | 0.35 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 13 | 0.35 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 13 | 0.35 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 13 | 0.35 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 13 | 0.35 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 13 | 0.35 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 13 | 0.35 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 20 | 0.35 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 20 | 0.35 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 20 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG2 | 19 | 0.35 |
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG3 | 19 | 0.35 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 19 | 0.35 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 19 | 0.35 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 5 | 0.35 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 5 | 0.35 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 5 | 0.35 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 13 | 0.35 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 13 | 0.35 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 13 | 0.35 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 2 | 0.35 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 2 | 0.35 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 17 | 0.35 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 17 | 0.35 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 8 | 0.35 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 8 | 0.35 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 8 | 0.35 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 7 | 0.35 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 7 | 0.35 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 7 | 0.35 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 3 | 0.35 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 3 | 0.35 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 3 | 0.35 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 19 | 0.35 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 19 | 0.35 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 19 | 0.35 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 8 | 0.35 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 8 | 0.35 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 8 | 0.35 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 12 | 0.35 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 12 | 0.35 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 12 | 0.35 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 15 | 0.35 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 15 | 0.35 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 15 | 0.35 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 9 | 0.35 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 3 | 0.35 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 10 | 0.35 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 10 | 0.35 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 10 | 0.35 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 6 | 0.35 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 6 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 6 | 0.35 |
| (1,191) | 1:152:A:LYS:H | 1:168:A:ALA:HA | 12 | 0.35 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 7 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 4 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 4 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 4 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 14 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 14 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 14 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 17 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 17 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 17 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 20 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 20 | 0.35 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 20 | 0.35 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 2 | 0.34 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 2 | 0.34 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 2 | 0.34 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 2 | 0.34 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 2 | 0.34 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 2 | 0.34 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 7 | 0.34 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 7 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD11 | 1:221:A:THR:HA | 5 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD12 | 1:221:A:THR:HA | 5 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD13 | 1:221:A:THR:HA | 5 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD21 | 1:221:A:THR:HA | 5 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD22 | 1:221:A:THR:HA | 5 | 0.34 |
| (1,3991) | 1:220:A:LEU:HD23 | 1:221:A:THR:HA | 5 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 19 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 19 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 19 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 19 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 19 | 0.34 |
| (1,3990) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 19 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 11 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 11 | 0.34 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 11 | 0.34 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 7 | 0.34 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 7 | 0.34 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 7 | 0.34 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 7 | 0.34 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 7 | 0.34 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 7 | 0.34 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 13 | 0.34 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 13 | 0.34 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 13 | 0.34 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 13 | 0.34 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 13 | 0.34 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 13 | 0.34 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 12 | 0.34 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 12 | 0.34 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD21 | 17 | 0.34 |
| (1,3858) | 1:148:A:SER:H | 1:175:A:ASN:HD22 | 17 | 0.34 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 19 | 0.34 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 19 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 14 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 14 | 0.34 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 14 | 0.34 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 7 | 0.34 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 7 | 0.34 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 7 | 0.34 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 7 | 0.34 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 7 | 0.34 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 7 | 0.34 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 18 | 0.34 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 18 | 0.34 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD21 | 17 | 0.34 |
| (1,3712) | 1:103:A:THR:HG21 | 1:129:A:ASN:HD22 | 17 | 0.34 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD21 | 17 | 0.34 |
| (1,3712) | 1:103:A:THR:HG22 | 1:129:A:ASN:HD22 | 17 | 0.34 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD21 | 17 | 0.34 |
| (1,3712) | 1:103:A:THR:HG23 | 1:129:A:ASN:HD22 | 17 | 0.34 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD21 | 20 | 0.34 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD22 | 20 | 0.34 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD21 | 20 | 0.34 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD22 | 20 | 0.34 |
| (1,3605) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HA | 7 | 0.34 |
| (1,3605) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HA | 7 | 0.34 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 14 | 0.34 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 14 | 0.34 |
| (1,3579) | 1:67:A:ALA:HA | 1:89:A:LEU:HD11 | 10 | 0.34 |
| (1,3579) | 1:67:A:ALA:HA | 1:89:A:LEU:HD12 | 10 | 0.34 |
| (1,3579) | 1:67:A:ALA:HA | 1:89:A:LEU:HD13 | 10 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3579) | 1:67:A:ALA:HA | 1:89:A:LEU:HD21 | 10 | 0.34 |
| (1,3579) | 1:67:A:ALA:HA | 1:89:A:LEU:HD22 | 10 | 0.34 |
| (1,3579) | 1:67:A:ALA:HA | 1:89:A:LEU:HD23 | 10 | 0.34 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG2 | 18 | 0.34 |
| (1,3554) | 1:55:A:ASN:HD21 | 1:76:A:MET:HG3 | 18 | 0.34 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 18 | 0.34 |
| (1,3554) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 18 | 0.34 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB2 | 3 | 0.34 |
| (1,3535) | 1:47:A:THR:HG21 | 1:48:A:ASN:HB3 | 3 | 0.34 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB2 | 3 | 0.34 |
| (1,3535) | 1:47:A:THR:HG22 | 1:48:A:ASN:HB3 | 3 | 0.34 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB2 | 3 | 0.34 |
| (1,3535) | 1:47:A:THR:HG23 | 1:48:A:ASN:HB3 | 3 | 0.34 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 11 | 0.34 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 11 | 0.34 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 16 | 0.34 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 16 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 11 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 11 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 11 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 11 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 11 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 11 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 17 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 17 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 17 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 17 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 17 | 0.34 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 17 | 0.34 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 20 | 0.34 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 20 | 0.34 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 20 | 0.34 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 8 | 0.34 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 8 | 0.34 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 8 | 0.34 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 13 | 0.34 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 13 | 0.34 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 13 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 11 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 11 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 11 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 11 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 17 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 17 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 17 | 0.34 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 17 | 0.34 |
| (1,3329) | 2:20:B:ARG:HD2 | 2:21:B:MET:H | 15 | 0.34 |
| (1,3329) | 2:20:B:ARG:HD3 | 2:21:B:MET:H | 15 | 0.34 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 15 | 0.34 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 8 | 0.34 |
| (1,3274) | 1:111:A:HIS:HD2 | 1:113:A:ASP:H | 14 | 0.34 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 15 | 0.34 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 8 | 0.34 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 2 | 0.34 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 2 | 0.34 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 2 | 0.34 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 6 | 0.34 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 6 | 0.34 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 6 | 0.34 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 14 | 0.34 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 14 | 0.34 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 14 | 0.34 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 13 | 0.34 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 13 | 0.34 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 5 | 0.34 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 5 | 0.34 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 17 | 0.34 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 9 | 0.34 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 12 | 0.34 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 5 | 0.34 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 11 | 0.34 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 13 | 0.34 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 11 | 0.34 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 11 | 0.34 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 11 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 6 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 6 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 6 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 10 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 10 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 10 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 11 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 11 | 0.34 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 11 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 9 | 0.34 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 16 | 0.34 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 4 | 0.34 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 7 | 0.34 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 9 | 0.34 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 9 | 0.34 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 9 | 0.34 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 7 | 0.34 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 1 | 0.34 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 4 | 0.34 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 4 | 0.34 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 4 | 0.34 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 11 | 0.34 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 11 | 0.34 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 11 | 0.34 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 6 | 0.34 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 10 | 0.34 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 11 | 0.34 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 11 | 0.34 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 11 | 0.34 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 11 | 0.34 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 11 | 0.34 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 11 | 0.34 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 1 | 0.34 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 1 | 0.34 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 1 | 0.34 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 1 | 0.34 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 19 | 0.34 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 3 | 0.34 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 3 | 0.34 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 3 | 0.34 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 7 | 0.34 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 7 | 0.34 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 7 | 0.34 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 15 | 0.34 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 12 | 0.34 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 12 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD11 | 1:131:A:LYS:H | 16 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD12 | 1:131:A:LYS:H | 16 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD13 | 1:131:A:LYS:H | 16 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD21 | 1:131:A:LYS:H | 16 | 0.34 |
| (1,2544) | 1:128:A:LEU:HD22 | 1:131:A:LYS:H | 16 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2544) | 1:128:A:LEU:HD23 | 1:131:A:LYS:H | 16 | 0.34 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 2 | 0.34 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 13 | 0.34 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 13 | 0.34 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 13 | 0.34 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 8 | 0.34 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 8 | 0.34 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 15 | 0.34 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG11 | 19 | 0.34 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG12 | 19 | 0.34 |
| (1,2442) | 1:114:A:ASP:H | 1:117:A:VAL:HG13 | 19 | 0.34 |
| (1,2437) | 1:82:A:LEU:HG | 1:113:A:ASP:H | 14 | 0.34 |
| (1,2376) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 20 | 0.34 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 18 | 0.34 |
| (1,2141) | 1:49:A:ASP:HA | 1:50:A:LEU:H | 15 | 0.34 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 18 | 0.34 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 18 | 0.34 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 18 | 0.34 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 19 | 0.34 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD11 | 15 | 0.34 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD12 | 15 | 0.34 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD13 | 15 | 0.34 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 13 | 0.34 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 13 | 0.34 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 13 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 11 | 0.34 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 11 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 6 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 6 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 6 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 11 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 11 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 11 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 18 | 0.34 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 18 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 18 | 0.34 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 14 | 0.34 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 14 | 0.34 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 14 | 0.34 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 10 | 0.34 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 10 | 0.34 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 2 | 0.34 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 2 | 0.34 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 16 | 0.34 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 6 | 0.34 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 12 | 0.34 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 12 | 0.34 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 12 | 0.34 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 8 | 0.34 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 8 | 0.34 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 2 | 0.34 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 2 | 0.34 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 2 | 0.34 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 14 | 0.34 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 14 | 0.34 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 14 | 0.34 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 20 | 0.34 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 20 | 0.34 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 20 | 0.34 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 10 | 0.34 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 10 | 0.34 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 10 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 11 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 11 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 11 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 11 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 11 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 11 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 14 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 14 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 14 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 14 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 14 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 14 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 20 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 20 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 20 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 20 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 20 | 0.34 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 20 | 0.34 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 9 | 0.34 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 9 | 0.34 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 9 | 0.34 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 9 | 0.34 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 9 | 0.34 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 9 | 0.34 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 9 | 0.34 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 3 | 0.34 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 12 | 0.34 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 12 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 7 | 0.34 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 7 | 0.34 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 15 | 0.34 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 13 | 0.34 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 13 | 0.34 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 15 | 0.34 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 15 | 0.34 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 15 | 0.34 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 15 | 0.34 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 15 | 0.34 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 15 | 0.34 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 16 | 0.34 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 16 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 16 | 0.34 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 16 | 0.34 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 16 | 0.34 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 16 | 0.34 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 8 | 0.34 |
| (1,1169) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 8 | 0.34 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 8 | 0.34 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 8 | 0.34 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 10 | 0.34 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 10 | 0.34 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 20 | 0.34 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 20 | 0.34 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 20 | 0.34 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 20 | 0.34 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 20 | 0.34 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 20 | 0.34 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 15 | 0.34 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 15 | 0.34 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 15 | 0.34 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 11 | 0.34 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 18 | 0.34 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 18 | 0.34 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 18 | 0.34 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 18 | 0.34 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 18 | 0.34 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 18 | 0.34 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 19 | 0.34 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 14 | 0.34 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 14 | 0.34 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 14 | 0.34 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 2 | 0.34 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 9 | 0.34 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 15 | 0.34 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 13 | 0.34 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 13 | 0.34 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 13 | 0.34 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 13 | 0.34 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 13 | 0.34 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 13 | 0.34 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 11 | 0.34 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 11 | 0.34 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 11 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 17 | 0.34 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 17 | 0.34 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 17 | 0.34 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 16 | 0.34 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 16 | 0.34 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 16 | 0.34 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 14 | 0.34 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 2 | 0.34 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 2 | 0.34 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 6 | 0.34 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 6 | 0.34 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 11 | 0.34 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 11 | 0.34 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 14 | 0.34 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 14 | 0.34 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 4 | 0.34 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 5 | 0.34 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 5 | 0.34 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 5 | 0.34 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 5 | 0.34 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 5 | 0.34 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 5 | 0.34 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG21 | 5 | 0.34 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG22 | 5 | 0.34 |
| (1,700) | 1:129:A:ASN:HB2 | 1:130:A:THR:HG23 | 5 | 0.34 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 17 | 0.34 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 17 | 0.34 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 20 | 0.34 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 20 | 0.34 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 20 | 0.34 |
| (1,591) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 15 | 0.34 |
| (1,475) | 1:82:A:LEU:HA | 1:112:A:TYR:HD1 | 1 | 0.34 |
| (1,475) | 1:82:A:LEU:HA | 1:112:A:TYR:HD2 | 1 | 0.34 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 5 | 0.34 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 5 | 0.34 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 5 | 0.34 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 11 | 0.34 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 11 | 0.34 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 11 | 0.34 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 18 | 0.34 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 18 | 0.34 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 18 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 20 | 0.34 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 20 | 0.34 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 20 | 0.34 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 13 | 0.34 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 3 | 0.34 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 19 | 0.34 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 1 | 0.34 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 1 | 0.34 |
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 1 | 0.34 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 1 | 0.34 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 1 | 0.34 |
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 1 | 0.34 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 18 | 0.34 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 18 | 0.34 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 18 | 0.34 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 19 | 0.34 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 19 | 0.34 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 19 | 0.34 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD11 | 2 | 0.34 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD12 | 2 | 0.34 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD13 | 2 | 0.34 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 6 | 0.34 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 6 | 0.34 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 6 | 0.34 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 7 | 0.34 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 7 | 0.34 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 7 | 0.34 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 9 | 0.33 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 9 | 0.33 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 9 | 0.33 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 9 | 0.33 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 9 | 0.33 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 9 | 0.33 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 16 | 0.33 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 16 | 0.33 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 16 | 0.33 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 16 | 0.33 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 16 | 0.33 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 16 | 0.33 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD21 | 4 | 0.33 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD22 | 4 | 0.33 |
| (1,3929) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD23 | 4 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD21 | 4 | 0.33 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD22 | 4 | 0.33 |
| (1,3929) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD23 | 4 | 0.33 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 1 | 0.33 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 1 | 0.33 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 1 | 0.33 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 1 | 0.33 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 1 | 0.33 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 1 | 0.33 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 18 | 0.33 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 18 | 0.33 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD21 | 10 | 0.33 |
| (1,3708) | 1:102:A:ARG:HG2 | 1:129:A:ASN:HD22 | 10 | 0.33 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD21 | 10 | 0.33 |
| (1,3708) | 1:102:A:ARG:HG3 | 1:129:A:ASN:HD22 | 10 | 0.33 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 19 | 0.33 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 19 | 0.33 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 19 | 0.33 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 19 | 0.33 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 19 | 0.33 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 19 | 0.33 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 3 | 0.33 |
| (1,3700) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 3 | 0.33 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 20 | 0.33 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 20 | 0.33 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 20 | 0.33 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 20 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 18 | 0.33 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 18 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 18 | 0.33 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 18 | 0.33 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 3 | 0.33 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 3 | 0.33 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 3 | 0.33 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 3 | 0.33 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 3 | 0.33 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 3 | 0.33 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 4 | 0.33 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 4 | 0.33 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 18 | 0.33 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 18 | 0.33 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 18 | 0.33 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 2 | 0.33 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 2 | 0.33 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 2 | 0.33 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 2 | 0.33 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 2 | 0.33 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 2 | 0.33 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 9 | 0.33 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 9 | 0.33 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 9 | 0.33 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 9 | 0.33 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 9 | 0.33 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 9 | 0.33 |
| (1,3474) | 2:17:B:LYS:HD2 | 2:18:B:CYS:H | 6 | 0.33 |
| (1,3474) | 2:17:B:LYS:HD3 | 2:18:B:CYS:H | 6 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 1 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 1 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 1 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 1 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 1 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 1 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 18 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 18 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 18 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 18 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 18 | 0.33 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 18 | 0.33 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 12 | 0.33 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 12 | 0.33 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 12 | 0.33 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD2 | 4 | 0.33 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD3 | 4 | 0.33 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD2 | 4 | 0.33 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD3 | 4 | 0.33 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD2 | 4 | 0.33 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD3 | 4 | 0.33 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 6 | 0.33 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 6 | 0.33 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 6 | 0.33 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 6 | 0.33 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 6 | 0.33 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 6 | 0.33 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 1 | 0.33 |
| (1,3283) | 1:69:A:PHE:HZ | 2:21:B:MET:HB2 | 19 | 0.33 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 2 | 0.33 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 7 | 0.33 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 7 | 0.33 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 7 | 0.33 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 19 | 0.33 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 19 | 0.33 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 19 | 0.33 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB1 | 12 | 0.33 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB2 | 12 | 0.33 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB3 | 12 | 0.33 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB1 | 12 | 0.33 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB2 | 12 | 0.33 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB3 | 12 | 0.33 |
| (1,3171) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HZ | 19 | 0.33 |
| (1,3171) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HZ | 19 | 0.33 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 11 | 0.33 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 11 | 0.33 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 11 | 0.33 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 18 | 0.33 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 8 | 0.33 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 16 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 7 | 0.33 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 5 | 0.33 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 5 | 0.33 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 5 | 0.33 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 15 | 0.33 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 7 | 0.33 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 7 | 0.33 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 7 | 0.33 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 2 | 0.33 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 2 | 0.33 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 2 | 0.33 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 3 | 0.33 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 18 | 0.33 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 18 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 2 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 2 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 2 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 5 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 5 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 5 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 7 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 7 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 7 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 14 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 14 | 0.33 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 14 | 0.33 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 10 | 0.33 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 9 | 0.33 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 13 | 0.33 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 3 | 0.33 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 3 | 0.33 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 3 | 0.33 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 8 | 0.33 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 17 | 0.33 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 12 | 0.33 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 12 | 0.33 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 12 | 0.33 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 16 | 0.33 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 16 | 0.33 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 16 | 0.33 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 5 | 0.33 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 5 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 5 | 0.33 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 5 | 0.33 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 5 | 0.33 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 5 | 0.33 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 10 | 0.33 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 8 | 0.33 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 8 | 0.33 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 8 | 0.33 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 19 | 0.33 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 19 | 0.33 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 19 | 0.33 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 15 | 0.33 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 15 | 0.33 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 15 | 0.33 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 18 | 0.33 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 18 | 0.33 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 18 | 0.33 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 6 | 0.33 |
| (1,2506) | 1:147:A:GLY:HA2 | 1:179:A:LEU:H | 3 | 0.33 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 12 | 0.33 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 20 | 0.33 |
| (1,2376) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 8 | 0.33 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 4 | 0.33 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 11 | 0.33 |
| (1,2120) | 1:74:A:ASP:HA | 1:83:A:GLN:HG3 | 20 | 0.33 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 8 | 0.33 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 13 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 12 | 0.33 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 12 | 0.33 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD11 | 20 | 0.33 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD12 | 20 | 0.33 |
| (1,1989) | 1:215:A:GLU:HG3 | 1:216:A:LEU:HD13 | 20 | 0.33 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 16 | 0.33 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 16 | 0.33 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 16 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 20 | 0.33 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 20 | 0.33 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 20 | 0.33 |
| (1,1877) | 1:202:A:THR:HA | 1:205:A:LYS:HG2 | 10 | 0.33 |
| (1,1814) | 1:123:A:LYS:HB2 | 1:136:A:TYR:H | 4 | 0.33 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 5 | 0.33 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 5 | 0.33 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 5 | 0.33 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 8 | 0.33 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 8 | 0.33 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 8 | 0.33 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 20 | 0.33 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 5 | 0.33 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 5 | 0.33 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 5 | 0.33 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 5 | 0.33 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 19 | 0.33 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE2 | 2 | 0.33 |
| (1,1586) | 1:196:A:ASN:HD22 | 1:225:A:LYS:HE3 | 2 | 0.33 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 6 | 0.33 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 6 | 0.33 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 6 | 0.33 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 18 | 0.33 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 18 | 0.33 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 18 | 0.33 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 16 | 0.33 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 14 | 0.33 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 14 | 0.33 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 14 | 0.33 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 5 | 0.33 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 5 | 0.33 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 3 | 0.33 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 3 | 0.33 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 3 | 0.33 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 3 | 0.33 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 18 | 0.33 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 18 | 0.33 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 14 | 0.33 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 11 | 0.33 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 11 | 0.33 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 11 | 0.33 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 11 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 11 | 0.33 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 14 | 0.33 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 14 | 0.33 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 19 | 0.33 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 19 | 0.33 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 15 | 0.33 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 15 | 0.33 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 15 | 0.33 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 3 | 0.33 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 9 | 0.33 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 2 | 0.33 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 2 | 0.33 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 2 | 0.33 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 2 | 0.33 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 2 | 0.33 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 2 | 0.33 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 1 | 0.33 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 18 | 0.33 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 18 | 0.33 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 18 | 0.33 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 7 | 0.33 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 9 | 0.33 |
| (1,1003) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HB3 | 4 | 0.33 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 10 | 0.33 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 12 | 0.33 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 17 | 0.33 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 20 | 0.33 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 8 | 0.33 |
| (1,969) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HA | 18 | 0.33 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 9 | 0.33 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE2 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HE3 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE2 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HE3 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE2 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HE3 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE2 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HE3 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE2 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HE3 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE2 | 3 | 0.33 |
| (1,944) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HE3 | 3 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 1 | 0.33 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 1 | 0.33 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 1 | 0.33 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 1 | 0.33 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 1 | 0.33 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 1 | 0.33 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 4 | 0.33 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 4 | 0.33 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 20 | 0.33 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 9 | 0.33 |
| (1,830) | 1:148:A:SER:H | 1:149:A:ALA:HB1 | 19 | 0.33 |
| (1,830) | 1:148:A:SER:H | 1:149:A:ALA:HB2 | 19 | 0.33 |
| (1,830) | 1:148:A:SER:H | 1:149:A:ALA:HB3 | 19 | 0.33 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 5 | 0.33 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 5 | 0.33 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 5 | 0.33 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 15 | 0.33 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 15 | 0.33 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 15 | 0.33 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 1 | 0.33 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 1 | 0.33 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 1 | 0.33 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 6 | 0.33 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 9 | 0.33 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 5 | 0.33 |
| (1,591) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 3 | 0.33 |
| (1,530) | 1:141:A:GLU:HA | 1:148:A:SER:HB2 | 19 | 0.33 |
| (1,530) | 1:141:A:GLU:HA | 1:148:A:SER:HB3 | 19 | 0.33 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB1 | 15 | 0.33 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB2 | 15 | 0.33 |
| (1,493) | 1:83:A:GLN:HG2 | 1:84:A:ALA:HB3 | 15 | 0.33 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 7 | 0.33 |
| (1,425) | 1:53:A:THR:HG21 | 1:76:A:MET:HG2 | 9 | 0.33 |
| (1,425) | 1:53:A:THR:HG21 | 1:76:A:MET:HG3 | 9 | 0.33 |
| (1,425) | 1:53:A:THR:HG22 | 1:76:A:MET:HG2 | 9 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,425) | 1:53:A:THR:HG22 | 1:76:A:MET:HG3 | 9 | 0.33 |
| (1,425) | 1:53:A:THR:HG23 | 1:76:A:MET:HG2 | 9 | 0.33 |
| (1,425) | 1:53:A:THR:HG23 | 1:76:A:MET:HG3 | 9 | 0.33 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 17 | 0.33 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 17 | 0.33 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 17 | 0.33 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 13 | 0.33 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 13 | 0.33 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 13 | 0.33 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 10 | 0.33 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 10 | 0.33 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 10 | 0.33 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 10 | 0.33 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 9 | 0.33 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 9 | 0.33 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 9 | 0.33 |
| (1,143) | 1:53:A:THR:HG21 | 1:55:A:ASN:HB3 | 8 | 0.33 |
| (1,143) | 1:53:A:THR:HG22 | 1:55:A:ASN:HB3 | 8 | 0.33 |
| (1,143) | 1:53:A:THR:HG23 | 1:55:A:ASN:HB3 | 8 | 0.33 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 12 | 0.33 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 12 | 0.33 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 12 | 0.33 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD11 | 2 | 0.33 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD12 | 2 | 0.33 |
| (1,70) | 1:216:A:LEU:H | 1:216:A:LEU:HD13 | 2 | 0.33 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 11 | 0.33 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 1 | 0.32 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 1 | 0.32 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 4 | 0.32 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 4 | 0.32 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 9 | 0.32 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 9 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 15 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 15 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 15 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 15 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 15 | 0.32 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 15 | 0.32 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 20 | 0.32 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 20 | 0.32 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 20 | 0.32 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 20 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 20 | 0.32 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 20 | 0.32 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 5 | 0.32 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 5 | 0.32 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 5 | 0.32 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 5 | 0.32 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 5 | 0.32 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 5 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 12 | 0.32 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 12 | 0.32 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 12 | 0.32 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 12 | 0.32 |
| (1,3717) | 1:105:A:ASP:HB2 | 1:126:A:ALA:H | 13 | 0.32 |
| (1,3717) | 1:105:A:ASP:HB3 | 1:126:A:ALA:H | 13 | 0.32 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 11 | 0.32 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 11 | 0.32 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 7 | 0.32 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB3 | 7 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 19 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 19 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 19 | 0.32 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 19 | 0.32 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 10 | 0.32 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 10 | 0.32 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 3 | 0.32 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 3 | 0.32 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 18 | 0.32 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 18 | 0.32 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 7 | 0.32 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 7 | 0.32 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB2 | 10 | 0.32 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 10 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB2 | 10 | 0.32 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 10 | 0.32 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB2 | 10 | 0.32 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 10 | 0.32 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG21 | 7 | 0.32 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG22 | 7 | 0.32 |
| (1,3545) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG23 | 7 | 0.32 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG21 | 7 | 0.32 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG22 | 7 | 0.32 |
| (1,3545) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG23 | 7 | 0.32 |
| (1,3508) | 1:51:A:PRO:HB2 | 2:7:B:PRO:HD2 | 8 | 0.32 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 3 | 0.32 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 3 | 0.32 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 3 | 0.32 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 3 | 0.32 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 3 | 0.32 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 3 | 0.32 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 16 | 0.32 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 16 | 0.32 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 16 | 0.32 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 16 | 0.32 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 16 | 0.32 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 16 | 0.32 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 16 | 0.32 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 16 | 0.32 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 16 | 0.32 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 16 | 0.32 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 16 | 0.32 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 16 | 0.32 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 20 | 0.32 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 20 | 0.32 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 16 | 0.32 |
| (1,3215) | 1:133:A:TRP:HZ2 | 1:140:A:ILE:HD11 | 19 | 0.32 |
| (1,3215) | 1:133:A:TRP:HZ2 | 1:140:A:ILE:HD12 | 19 | 0.32 |
| (1,3215) | 1:133:A:TRP:HZ2 | 1:140:A:ILE:HD13 | 19 | 0.32 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 2 | 0.32 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 2 | 0.32 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 2 | 0.32 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 2 | 0.32 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 2 | 0.32 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 2 | 0.32 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 14 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 14 | 0.32 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 14 | 0.32 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 14 | 0.32 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 14 | 0.32 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 14 | 0.32 |
| (1,3160) | 1:133:A:TRP:HH2 | 1:135:A:PHE:HD1 | 19 | 0.32 |
| (1,3160) | 1:133:A:TRP:HH2 | 1:135:A:PHE:HD2 | 19 | 0.32 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 17 | 0.32 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 17 | 0.32 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 7 | 0.32 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 14 | 0.32 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 7 | 0.32 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 19 | 0.32 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 19 | 0.32 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 19 | 0.32 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 12 | 0.32 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 15 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 6 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 6 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 7 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 7 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 13 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 13 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 14 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 14 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 17 | 0.32 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 17 | 0.32 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 8 | 0.32 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 8 | 0.32 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 8 | 0.32 |
| (1,3000) | 1:212:A:LYS:H | 1:212:A:LYS:HE3 | 12 | 0.32 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 3 | 0.32 |
| (1,2977) | 1:205:A:LYS:HG2 | 1:206:A:ALA:H | 11 | 0.32 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 8 | 0.32 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 11 | 0.32 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 9 | 0.32 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 17 | 0.32 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 17 | 0.32 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 17 | 0.32 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 19 | 0.32 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 19 | 0.32 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 19 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 11 | 0.32 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 11 | 0.32 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 11 | 0.32 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 20 | 0.32 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 13 | 0.32 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 2 | 0.32 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 4 | 0.32 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 14 | 0.32 |
| (1,2638) | 1:142:A:THR:HG21 | 1:147:A:GLY:H | 19 | 0.32 |
| (1,2638) | 1:142:A:THR:HG22 | 1:147:A:GLY:H | 19 | 0.32 |
| (1,2638) | 1:142:A:THR:HG23 | 1:147:A:GLY:H | 19 | 0.32 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 2 | 0.32 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 2 | 0.32 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 2 | 0.32 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 9 | 0.32 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 15 | 0.32 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 15 | 0.32 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 10 | 0.32 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 1 | 0.32 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 5 | 0.32 |
| (1,2217) | 1:62:A:ASP:H | 1:66:A:ASP:HB2 | 2 | 0.32 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 11 | 0.32 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 16 | 0.32 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 16 | 0.32 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 16 | 0.32 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 3 | 0.32 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 3 | 0.32 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 2 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 3 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 3 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 9 | 0.32 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 9 | 0.32 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 5 | 0.32 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 17 | 0.32 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 17 | 0.32 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 17 | 0.32 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 12 | 0.32 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 12 | 0.32 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 12 | 0.32 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 12 | 0.32 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 12 | 0.32 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 12 | 0.32 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 1 | 0.32 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 1 | 0.32 |
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 1 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 17 | 0.32 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 17 | 0.32 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 8 | 0.32 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 8 | 0.32 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 8 | 0.32 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 9 | 0.32 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 9 | 0.32 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 9 | 0.32 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 17 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 17 | 0.32 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 11 | 0.32 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 11 | 0.32 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 11 | 0.32 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 11 | 0.32 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 11 | 0.32 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 11 | 0.32 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 6 | 0.32 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 17 | 0.32 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 17 | 0.32 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 17 | 0.32 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 3 | 0.32 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 3 | 0.32 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 3 | 0.32 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 11 | 0.32 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 7 | 0.32 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 7 | 0.32 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 7 | 0.32 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 18 | 0.32 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 18 | 0.32 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 18 | 0.32 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 1 | 0.32 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 1 | 0.32 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 1 | 0.32 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 11 | 0.32 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 11 | 0.32 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 11 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD11 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD12 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD13 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD11 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD12 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD13 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD11 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD12 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD13 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD11 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD12 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD13 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD11 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD12 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD13 | 14 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD11 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD12 | 14 | 0.32 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD13 | 14 | 0.32 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 18 | 0.32 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 18 | 0.32 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 18 | 0.32 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 18 | 0.32 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 18 | 0.32 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 18 | 0.32 |
| (1,1422) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HA | 12 | 0.32 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 20 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 2 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 2 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 2 | 0.32 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 2 | 0.32 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 18 | 0.32 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 18 | 0.32 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 18 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 1 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 1 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 1 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 16 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 16 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 16 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 20 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 20 | 0.32 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 20 | 0.32 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 4 | 0.32 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 20 | 0.32 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 20 | 0.32 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 20 | 0.32 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 20 | 0.32 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 20 | 0.32 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 20 | 0.32 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 20 | 0.32 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 20 | 0.32 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 20 | 0.32 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 19 | 0.32 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 19 | 0.32 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 19 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 13 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 13 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 13 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 14 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 14 | 0.32 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 14 | 0.32 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 6 | 0.32 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 6 | 0.32 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 6 | 0.32 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 6 | 0.32 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 6 | 0.32 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 6 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 2 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 2 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 2 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 2 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 2 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 2 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 12 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 12 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 12 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 12 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 12 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 12 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 14 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 14 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 14 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 14 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 14 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 14 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 16 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 16 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 16 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 16 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 16 | 0.32 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 16 | 0.32 |
| (1,1089) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HB3 | 5 | 0.32 |
| (1,1089) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HB3 | 5 | 0.32 |
| (1,1089) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HB3 | 5 | 0.32 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 3 | 0.32 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 3 | 0.32 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 3 | 0.32 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 14 | 0.32 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 14 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 14 | 0.32 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 2 | 0.32 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 6 | 0.32 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 18 | 0.32 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 18 | 0.32 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE2 | 5 | 0.32 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE3 | 5 | 0.32 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 18 | 0.32 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 18 | 0.32 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 18 | 0.32 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 6 | 0.32 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 9 | 0.32 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 9 | 0.32 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 9 | 0.32 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 20 | 0.32 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 10 | 0.32 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 9 | 0.32 |
| (1,698) | 1:106:A:ALA:HB1 | 1:124:A:GLY:HA2 | 20 | 0.32 |
| (1,698) | 1:106:A:ALA:HB2 | 1:124:A:GLY:HA2 | 20 | 0.32 |
| (1,698) | 1:106:A:ALA:HB3 | 1:124:A:GLY:HA2 | 20 | 0.32 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 2 | 0.32 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 2 | 0.32 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 15 | 0.32 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 15 | 0.32 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 18 | 0.32 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 18 | 0.32 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 18 | 0.32 |
| (1,591) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 17 | 0.32 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 13 | 0.32 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 11 | 0.32 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 5 | 0.32 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 9 | 0.32 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 12 | 0.32 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 12 | 0.32 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 9 | 0.32 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 14 | 0.32 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 14 | 0.32 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 14 | 0.32 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 12 | 0.32 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 6 | 0.32 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 6 | 0.32 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 6 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 1 | 0.32 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 1 | 0.32 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 1 | 0.32 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 6 | 0.32 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 6 | 0.32 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 6 | 0.32 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 6 | 0.32 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 6 | 0.32 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 6 | 0.32 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 6 | 0.32 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 6 | 0.32 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 6 | 0.32 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 9 | 0.32 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 9 | 0.32 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 9 | 0.32 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 10 | 0.32 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 10 | 0.32 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 10 | 0.32 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 8 | 0.32 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 8 | 0.32 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 8 | 0.32 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 13 | 0.32 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 13 | 0.32 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 13 | 0.32 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 6 | 0.32 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 6 | 0.32 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 19 | 0.32 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 19 | 0.32 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 19 | 0.32 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 20 | 0.32 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 20 | 0.32 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 20 | 0.32 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 5 | 0.31 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 5 | 0.31 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 5 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 5 | 0.31 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 5 | 0.31 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 5 | 0.31 |
| (1,3991) | 1:220:A:LEU:HD11 | 1:221:A:THR:HA | 3 | 0.31 |
| (1,3991) | 1:220:A:LEU:HD12 | 1:221:A:THR:HA | 3 | 0.31 |
| (1,3991) | 1:220:A:LEU:HD13 | 1:221:A:THR:HA | 3 | 0.31 |
| (1,3991) | 1:220:A:LEU:HD21 | 1:221:A:THR:HA | 3 | 0.31 |
| (1,3991) | 1:220:A:LEU:HD22 | 1:221:A:THR:HA | 3 | 0.31 |
| (1,3991) | 1:220:A:LEU:HD23 | 1:221:A:THR:HA | 3 | 0.31 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 16 | 0.31 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 16 | 0.31 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 3 | 0.31 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 3 | 0.31 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 3 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 5 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 5 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 20 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 20 | 0.31 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 20 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 19 | 0.31 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 19 | 0.31 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 3 | 0.31 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 3 | 0.31 |
| (1,3682) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 15 | 0.31 |
| (1,3682) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 15 | 0.31 |
| (1,3682) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 20 | 0.31 |
| (1,3682) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 20 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 4 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 4 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 4 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 4 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 10 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 10 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 10 | 0.31 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 10 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 15 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 15 | 0.31 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 15 | 0.31 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 4 | 0.31 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB3 | 4 | 0.31 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 18 | 0.31 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 18 | 0.31 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 18 | 0.31 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 18 | 0.31 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 20 | 0.31 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 20 | 0.31 |
| (1,3521) | 1:59:A:ALA:HB1 | 2:12:B:ASN:HB2 | 3 | 0.31 |
| (1,3521) | 1:59:A:ALA:HB2 | 2:12:B:ASN:HB2 | 3 | 0.31 |
| (1,3521) | 1:59:A:ALA:HB3 | 2:12:B:ASN:HB2 | 3 | 0.31 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 9 | 0.31 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 7 | 0.31 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 7 | 0.31 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 7 | 0.31 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 13 | 0.31 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 13 | 0.31 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 13 | 0.31 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 17 | 0.31 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 17 | 0.31 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 17 | 0.31 |
| (1,3396) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HA | 10 | 0.31 |
| (1,3396) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HA | 10 | 0.31 |
| (1,3396) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HA | 10 | 0.31 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 14 | 0.31 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 14 | 0.31 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 15 | 0.31 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 15 | 0.31 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 15 | 0.31 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 15 | 0.31 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 6 | 0.31 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 6 | 0.31 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 6 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 2 | 0.31 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 12 | 0.31 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 12 | 0.31 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 12 | 0.31 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 15 | 0.31 |
| (1,3068) | 1:195:A:ASN:HA | 1:196:A:ASN:HD21 | 11 | 0.31 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 11 | 0.31 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 17 | 0.31 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 9 | 0.31 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 9 | 0.31 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 9 | 0.31 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 19 | 0.31 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 1 | 0.31 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 1 | 0.31 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 2 | 0.31 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 2 | 0.31 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 9 | 0.31 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 9 | 0.31 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 9 | 0.31 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 8 | 0.31 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 16 | 0.31 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 20 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 4 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 4 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 4 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 5 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 5 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 5 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 8 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 8 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 8 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 11 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 11 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 11 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 13 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 13 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 13 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 14 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 14 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 14 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 15 | 0.31 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 15 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 15 | 0.31 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 5 | 0.31 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 9 | 0.31 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 18 | 0.31 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 12 | 0.31 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 12 | 0.31 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 12 | 0.31 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 4 | 0.31 |
| (1,2761) | 1:167:A:ASP:H | 1:196:A:ASN:HB2 | 5 | 0.31 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 3 | 0.31 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 3 | 0.31 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 3 | 0.31 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 3 | 0.31 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 20 | 0.31 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 20 | 0.31 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 20 | 0.31 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 18 | 0.31 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 19 | 0.31 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 1 | 0.31 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 1 | 0.31 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 1 | 0.31 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 1 | 0.31 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 1 | 0.31 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 1 | 0.31 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 8 | 0.31 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 16 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 13 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 13 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 13 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 17 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 17 | 0.31 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 17 | 0.31 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 18 | 0.31 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 18 | 0.31 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 18 | 0.31 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 4 | 0.31 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 17 | 0.31 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 19 | 0.31 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 19 | 0.31 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 19 | 0.31 |
| (1,2443) | 1:114:A:ASP:H | 1:143:A:VAL:HG21 | 5 | 0.31 |
| (1,2443) | 1:114:A:ASP:H | 1:143:A:VAL:HG22 | 5 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2443) | 1:114:A:ASP:H | 1:143:A:VAL:HG23 | 5 | 0.31 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 9 | 0.31 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 3 | 0.31 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 16 | 0.31 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 16 | 0.31 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD2 | 18 | 0.31 |
| (1,2102) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HD3 | 18 | 0.31 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 16 | 0.31 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 10 | 0.31 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG21 | 12 | 0.31 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG22 | 12 | 0.31 |
| (1,2063) | 1:206:A:ALA:H | 1:222:A:ILE:HG23 | 12 | 0.31 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 11 | 0.31 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 11 | 0.31 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 11 | 0.31 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD11 | 13 | 0.31 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD12 | 13 | 0.31 |
| (1,2011) | 1:185:A:LYS:H | 1:216:A:LEU:HD13 | 13 | 0.31 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD11 | 13 | 0.31 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD12 | 13 | 0.31 |
| (1,2005) | 1:185:A:LYS:HA | 1:216:A:LEU:HD13 | 13 | 0.31 |
| (1,2002) | 1:216:A:LEU:H | 1:216:A:LEU:HG | 19 | 0.31 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 8 | 0.31 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 5 | 0.31 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 5 | 0.31 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 5 | 0.31 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 19 | 0.31 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 19 | 0.31 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 19 | 0.31 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 3 | 0.31 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 3 | 0.31 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 3 | 0.31 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 5 | 0.31 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 5 | 0.31 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 5 | 0.31 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 20 | 0.31 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 20 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 10 | 0.31 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 10 | 0.31 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 10 | 0.31 |
| (1,1739) | 1:197:A:ALA:HA | 1:225:A:LYS:HB3 | 4 | 0.31 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 5 | 0.31 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 14 | 0.31 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 7 | 0.31 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 19 | 0.31 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 14 | 0.31 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 14 | 0.31 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 14 | 0.31 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 11 | 0.31 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 11 | 0.31 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 11 | 0.31 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 15 | 0.31 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 15 | 0.31 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 15 | 0.31 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 14 | 0.31 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 16 | 0.31 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 16 | 0.31 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 16 | 0.31 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 6 | 0.31 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 6 | 0.31 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 6 | 0.31 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 17 | 0.31 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 17 | 0.31 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 17 | 0.31 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 4 | 0.31 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 4 | 0.31 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 4 | 0.31 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 12 | 0.31 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 12 | 0.31 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 12 | 0.31 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 8 | 0.31 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 8 | 0.31 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 8 | 0.31 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 8 | 0.31 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 8 | 0.31 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 8 | 0.31 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 12 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 12 | 0.31 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 6 | 0.31 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 10 | 0.31 |
| (1,1380) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB2 | 9 | 0.31 |
| (1,1380) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB2 | 9 | 0.31 |
| (1,1380) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB2 | 9 | 0.31 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 2 | 0.31 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 14 | 0.31 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 9 | 0.31 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 9 | 0.31 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 9 | 0.31 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 14 | 0.31 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 14 | 0.31 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 14 | 0.31 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 19 | 0.31 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 14 | 0.31 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 14 | 0.31 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 14 | 0.31 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 14 | 0.31 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 11 | 0.31 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 11 | 0.31 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 11 | 0.31 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 5 | 0.31 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 1 | 0.31 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 1 | 0.31 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 1 | 0.31 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 1 | 0.31 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 1 | 0.31 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 1 | 0.31 |
| (1,1146) | 1:142:A:THR:HA | 1:147:A:GLY:HA3 | 5 | 0.31 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 4 | 0.31 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 4 | 0.31 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 4 | 0.31 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 5 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 1 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 1 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 1 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 1 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 1 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 1 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 11 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 11 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 11 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 11 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 11 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 11 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 13 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 13 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 13 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 13 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 13 | 0.31 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 13 | 0.31 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 12 | 0.31 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 18 | 0.31 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 6 | 0.31 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 6 | 0.31 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 6 | 0.31 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 6 | 0.31 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 6 | 0.31 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 6 | 0.31 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 4 | 0.31 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 13 | 0.31 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 16 | 0.31 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 16 | 0.31 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 16 | 0.31 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 1 | 0.31 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 6 | 0.31 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 10 | 0.31 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD21 | 13 | 0.31 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD22 | 13 | 0.31 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD23 | 13 | 0.31 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 11 | 0.31 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 11 | 0.31 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 11 | 0.31 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 13 | 0.31 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 13 | 0.31 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 13 | 0.31 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 2 | 0.31 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 2 | 0.31 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 2 | 0.31 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 2 | 0.31 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 2 | 0.31 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 2 | 0.31 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 13 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 13 | 0.31 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 13 | 0.31 |
| (1,769) | 1:82:A:LEU:HG | 1:112:A:TYR:HA | 14 | 0.31 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 12 | 0.31 |
| (1,655) | 1:102:A:ARG:HD2 | 1:103:A:THR:H | 13 | 0.31 |
| (1,655) | 1:102:A:ARG:HD3 | 1:103:A:THR:H | 13 | 0.31 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 15 | 0.31 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 19 | 0.31 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 15 | 0.31 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 15 | 0.31 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 15 | 0.31 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 15 | 0.31 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 15 | 0.31 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 15 | 0.31 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 17 | 0.31 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 17 | 0.31 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 17 | 0.31 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 5 | 0.31 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 13 | 0.31 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 17 | 0.31 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 7 | 0.31 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 7 | 0.31 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 7 | 0.31 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 3 | 0.31 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 3 | 0.31 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 3 | 0.31 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 15 | 0.31 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 15 | 0.31 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 15 | 0.31 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 3 | 0.31 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 3 | 0.31 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 3 | 0.31 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 3 | 0.31 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 3 | 0.31 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 3 | 0.31 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 10 | 0.31 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 10 | 0.31 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 10 | 0.31 |
| (1,344) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HA | 8 | 0.31 |
| (1,344) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HA | 8 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 4 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 4 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 4 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 7 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 7 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 7 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 20 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 20 | 0.31 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 20 | 0.31 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 13 | 0.31 |
| (1,4047) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB2 | 16 | 0.3 |
| (1,4047) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB2 | 16 | 0.3 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG2 | 13 | 0.3 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG3 | 13 | 0.3 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG2 | 13 | 0.3 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG3 | 13 | 0.3 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG2 | 13 | 0.3 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG3 | 13 | 0.3 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG2 | 9 | 0.3 |
| (1,4009) | 2:10:B:TYR:H | 2:21:B:MET:HG3 | 9 | 0.3 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 3 | 0.3 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 3 | 0.3 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD11 | 3 | 0.3 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD12 | 3 | 0.3 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD13 | 3 | 0.3 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 3 | 0.3 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 3 | 0.3 |
| (1,3970) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 3 | 0.3 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 4 | 0.3 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 4 | 0.3 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 4 | 0.3 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 4 | 0.3 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 4 | 0.3 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 4 | 0.3 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 7 | 0.3 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 7 | 0.3 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 7 | 0.3 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 7 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 7 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 7 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 7 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 7 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 7 | 0.3 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 7 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 2 | 0.3 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 2 | 0.3 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 2 | 0.3 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 2 | 0.3 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 2 | 0.3 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 2 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 16 | 0.3 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 16 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 19 | 0.3 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 19 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 10 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 10 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 15 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 15 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 18 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 18 | 0.3 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 18 | 0.3 |
| (1,3791) | 1:119:A:LEU:HD11 | 1:133:A:TRP:HE1 | 19 | 0.3 |
| (1,3791) | 1:119:A:LEU:HD12 | 1:133:A:TRP:HE1 | 19 | 0.3 |
| (1,3791) | 1:119:A:LEU:HD13 | 1:133:A:TRP:HE1 | 19 | 0.3 |
| (1,3791) | 1:119:A:LEU:HD21 | 1:133:A:TRP:HE1 | 19 | 0.3 |
| (1,3791) | 1:119:A:LEU:HD22 | 1:133:A:TRP:HE1 | 19 | 0.3 |
| (1,3791) | 1:119:A:LEU:HD23 | 1:133:A:TRP:HE1 | 19 | 0.3 |
| (1,3737) | 1:110:A:VAL:HG11 | 1:120:A:LYS:H | 5 | 0.3 |
| (1,3737) | 1:110:A:VAL:HG12 | 1:120:A:LYS:H | 5 | 0.3 |
| (1,3737) | 1:110:A:VAL:HG13 | 1:120:A:LYS:H | 5 | 0.3 |
| (1,3737) | 1:110:A:VAL:HG21 | 1:120:A:LYS:H | 5 | 0.3 |
| (1,3737) | 1:110:A:VAL:HG22 | 1:120:A:LYS:H | 5 | 0.3 |
| (1,3737) | 1:110:A:VAL:HG23 | 1:120:A:LYS:H | 5 | 0.3 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 1 | 0.3 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 1 | 0.3 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 7 | 0.3 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 7 | 0.3 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG21 | 20 | 0.3 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG22 | 20 | 0.3 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG23 | 20 | 0.3 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG21 | 20 | 0.3 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG22 | 20 | 0.3 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG23 | 20 | 0.3 |
| (1,3682) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 3 | 0.3 |
| (1,3682) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 3 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 6 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 6 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 6 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 6 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 11 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 11 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 11 | 0.3 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 11 | 0.3 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 18 | 0.3 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB3 | 18 | 0.3 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 15 | 0.3 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 15 | 0.3 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 17 | 0.3 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 17 | 0.3 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB2 | 17 | 0.3 |
| (1,3560) | 1:61:A:GLY:HA2 | 1:66:A:ASP:HB3 | 17 | 0.3 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB2 | 17 | 0.3 |
| (1,3560) | 1:61:A:GLY:HA3 | 1:66:A:ASP:HB3 | 17 | 0.3 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 6 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 1 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 1 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 1 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 1 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 1 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 1 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 11 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 11 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 11 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 11 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 11 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 11 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 13 | 0.3 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 13 | 0.3 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 4 | 0.3 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 4 | 0.3 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 4 | 0.3 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 8 | 0.3 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 8 | 0.3 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 8 | 0.3 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 19 | 0.3 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 19 | 0.3 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 6 | 0.3 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 6 | 0.3 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 6 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3411) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB2 | 16 | 0.3 |
| (1,3411) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB2 | 16 | 0.3 |
| (1,3411) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB2 | 16 | 0.3 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 6 | 0.3 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 6 | 0.3 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 18 | 0.3 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 18 | 0.3 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 8 | 0.3 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 8 | 0.3 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 15 | 0.3 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 15 | 0.3 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 15 | 0.3 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 19 | 0.3 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 15 | 0.3 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 16 | 0.3 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 16 | 0.3 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 16 | 0.3 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 16 | 0.3 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 16 | 0.3 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 16 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 2 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 2 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 18 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 18 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 19 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 19 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 20 | 0.3 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 20 | 0.3 |
| (1,3139) | 1:82:A:LEU:HB2 | 1:112:A:TYR:HD1 | 12 | 0.3 |
| (1,3139) | 1:82:A:LEU:HB2 | 1:112:A:TYR:HD2 | 12 | 0.3 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 2 | 0.3 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 2 | 0.3 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 2 | 0.3 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 18 | 0.3 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 19 | 0.3 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 3 | 0.3 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 3 | 0.3 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 3 | 0.3 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 9 | 0.3 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 9 | 0.3 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 11 | 0.3 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 11 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 16 | 0.3 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 16 | 0.3 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 16 | 0.3 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 16 | 0.3 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 16 | 0.3 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 20 | 0.3 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 20 | 0.3 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 20 | 0.3 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 2 | 0.3 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 2 | 0.3 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 6 | 0.3 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 14 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 6 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 6 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 6 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 9 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 9 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 9 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 16 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 16 | 0.3 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 16 | 0.3 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 10 | 0.3 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 10 | 0.3 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 10 | 0.3 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 4 | 0.3 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 4 | 0.3 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 20 | 0.3 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 2 | 0.3 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 2 | 0.3 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 2 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 2 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 2 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 2 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 6 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 6 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 6 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 7 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 7 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 7 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 10 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 10 | 0.3 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 10 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 20 | 0.3 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 10 | 0.3 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 10 | 0.3 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 10 | 0.3 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 8 | 0.3 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 12 | 0.3 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 12 | 0.3 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 12 | 0.3 |
| (1,2506) | 1:147:A:GLY:HA2 | 1:179:A:LEU:H | 5 | 0.3 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 15 | 0.3 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 16 | 0.3 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 3 | 0.3 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 3 | 0.3 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 9 | 0.3 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 15 | 0.3 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD21 | 7 | 0.3 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD22 | 7 | 0.3 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD23 | 7 | 0.3 |
| (1,2016) | 1:190:A:LYS:HG3 | 1:218:A:ALA:HA | 2 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 10 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 20 | 0.3 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 20 | 0.3 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 1 | 0.3 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 1 | 0.3 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 1 | 0.3 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 15 | 0.3 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 15 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 15 | 0.3 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 18 | 0.3 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 18 | 0.3 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 18 | 0.3 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 13 | 0.3 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 13 | 0.3 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 13 | 0.3 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 19 | 0.3 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 19 | 0.3 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 19 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 8 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 8 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 15 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 15 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 16 | 0.3 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 16 | 0.3 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 2 | 0.3 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 3 | 0.3 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 13 | 0.3 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 13 | 0.3 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 13 | 0.3 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 9 | 0.3 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 9 | 0.3 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 9 | 0.3 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 20 | 0.3 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 8 | 0.3 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 13 | 0.3 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 20 | 0.3 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 20 | 0.3 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 20 | 0.3 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 20 | 0.3 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 1 | 0.3 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 1 | 0.3 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 1 | 0.3 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 3 | 0.3 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 3 | 0.3 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 3 | 0.3 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 14 | 0.3 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 14 | 0.3 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 14 | 0.3 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 17 | 0.3 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 17 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 17 | 0.3 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 17 | 0.3 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 17 | 0.3 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 17 | 0.3 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 15 | 0.3 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 15 | 0.3 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 15 | 0.3 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 15 | 0.3 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 15 | 0.3 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 15 | 0.3 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 4 | 0.3 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 12 | 0.3 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 20 | 0.3 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 1 | 0.3 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 4 | 0.3 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 4 | 0.3 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 14 | 0.3 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 14 | 0.3 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 9 | 0.3 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 9 | 0.3 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 9 | 0.3 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 17 | 0.3 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 17 | 0.3 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 17 | 0.3 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 19 | 0.3 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 19 | 0.3 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 19 | 0.3 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 14 | 0.3 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 2 | 0.3 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 2 | 0.3 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 2 | 0.3 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 2 | 0.3 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 2 | 0.3 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 2 | 0.3 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 1 | 0.3 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 1 | 0.3 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 1 | 0.3 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 3 | 0.3 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 3 | 0.3 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 3 | 0.3 |
| (1,1119) | 1:142:A:THR:HB | 1:183:A:ALA:H | 19 | 0.3 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 4 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 4 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 4 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 4 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 4 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 4 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 15 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 15 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 15 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 15 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 15 | 0.3 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 15 | 0.3 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 17 | 0.3 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 17 | 0.3 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 17 | 0.3 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 4 | 0.3 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 4 | 0.3 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 4 | 0.3 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 11 | 0.3 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 11 | 0.3 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 11 | 0.3 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 5 | 0.3 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 5 | 0.3 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 8 | 0.3 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 14 | 0.3 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 15 | 0.3 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 15 | 0.3 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 15 | 0.3 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 4 | 0.3 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 4 | 0.3 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 4 | 0.3 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 4 | 0.3 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 4 | 0.3 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 4 | 0.3 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 20 | 0.3 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 20 | 0.3 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 20 | 0.3 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 20 | 0.3 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 20 | 0.3 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 20 | 0.3 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 20 | 0.3 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 20 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 20 | 0.3 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 8 | 0.3 |
| (1,729) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 20 | 0.3 |
| (1,613) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG2 | 20 | 0.3 |
| (1,613) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG2 | 20 | 0.3 |
| (1,613) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG2 | 20 | 0.3 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 12 | 0.3 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 12 | 0.3 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 12 | 0.3 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 12 | 0.3 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 12 | 0.3 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 12 | 0.3 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 14 | 0.3 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 4 | 0.3 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 14 | 0.3 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 7 | 0.3 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 7 | 0.3 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 7 | 0.3 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 5 | 0.3 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 5 | 0.3 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 5 | 0.3 |
| (1,416) | 1:125:A:TRP:HE3 | 1:155:A:LYS:HA | 18 | 0.3 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 5 | 0.3 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 5 | 0.3 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 5 | 0.3 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 5 | 0.3 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 5 | 0.3 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 5 | 0.3 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 5 | 0.3 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 5 | 0.3 |
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 5 | 0.3 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 5 | 0.3 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 5 | 0.3 |
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 5 | 0.3 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 12 | 0.3 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 12 | 0.3 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 12 | 0.3 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 2 | 0.3 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 2 | 0.3 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 2 | 0.3 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 7 | 0.3 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 7 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 7 | 0.3 |
| (1,146) | 1:55:A:ASN:HB3 | 2:12:B:ASN:H | 13 | 0.3 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 17 | 0.3 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 17 | 0.3 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 17 | 0.3 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 8 | 0.3 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 14 | 0.3 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 19 | 0.3 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 19 | 0.3 |
| (1,17) | 1:47:A:THR:HG21 | 1:48:A:ASN:H | 7 | 0.3 |
| (1,17) | 1:47:A:THR:HG22 | 1:48:A:ASN:H | 7 | 0.3 |
| (1,17) | 1:47:A:THR:HG23 | 1:48:A:ASN:H | 7 | 0.3 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB2 | 3 | 0.29 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB3 | 3 | 0.29 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB2 | 3 | 0.29 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB3 | 3 | 0.29 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB2 | 3 | 0.29 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB3 | 3 | 0.29 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 9 | 0.29 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 9 | 0.29 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 17 | 0.29 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 17 | 0.29 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 6 | 0.29 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 6 | 0.29 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 5 | 0.29 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 5 | 0.29 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 5 | 0.29 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 5 | 0.29 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 5 | 0.29 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 5 | 0.29 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 9 | 0.29 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 9 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD11 | 14 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD12 | 14 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD13 | 14 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 14 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 14 | 0.29 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 14 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD11 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD12 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD13 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD21 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD22 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HD23 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD11 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD12 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD13 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD21 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD22 | 6 | 0.29 |
| (1,3715) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HD23 | 6 | 0.29 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 5 | 0.29 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 5 | 0.29 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 10 | 0.29 |
| (1,3685) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 10 | 0.29 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 10 | 0.29 |
| (1,3685) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 10 | 0.29 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 10 | 0.29 |
| (1,3685) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 10 | 0.29 |
| (1,3682) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 8 | 0.29 |
| (1,3682) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 8 | 0.29 |
| (1,3682) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 17 | 0.29 |
| (1,3682) | 1:93:A:GLU:HB3 | 1:94:A:ALA:H | 17 | 0.29 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 13 | 0.29 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 13 | 0.29 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 18 | 0.29 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 18 | 0.29 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 18 | 0.29 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 18 | 0.29 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 20 | 0.29 |
| (1,3505) | 1:51:A:PRO:HB3 | 2:7:B:PRO:HD3 | 19 | 0.29 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 18 | 0.29 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 18 | 0.29 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 18 | 0.29 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 10 | 0.29 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 10 | 0.29 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 16 | 0.29 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 16 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 16 | 0.29 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 3 | 0.29 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 3 | 0.29 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 3 | 0.29 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 3 | 0.29 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 3 | 0.29 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 3 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 15 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 15 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 15 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 17 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 17 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 17 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 20 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 20 | 0.29 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 20 | 0.29 |
| (1,3406) | 2:8:B:ILE:HD11 | 2:21:B:MET:HG3 | 6 | 0.29 |
| (1,3406) | 2:8:B:ILE:HD12 | 2:21:B:MET:HG3 | 6 | 0.29 |
| (1,3406) | 2:8:B:ILE:HD13 | 2:21:B:MET:HG3 | 6 | 0.29 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 17 | 0.29 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 4 | 0.29 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 4 | 0.29 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 1 | 0.29 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 6 | 0.29 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 16 | 0.29 |
| (1,3249) | 1:143:A:VAL:HB | 1:182:A:HIS:HE1 | 17 | 0.29 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 5 | 0.29 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 5 | 0.29 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 5 | 0.29 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 5 | 0.29 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 5 | 0.29 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 5 | 0.29 |
| (1,3120) | 1:63:A:TYR:HE1 | 1:64:A:PRO:HB3 | 19 | 0.29 |
| (1,3120) | 1:63:A:TYR:HE2 | 1:64:A:PRO:HB3 | 19 | 0.29 |
| (1,3091) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 16 | 0.29 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 10 | 0.29 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 2 | 0.29 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 6 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 3 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 3 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 3 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 17 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 17 | 0.29 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 17 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 8 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 8 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 8 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 15 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 15 | 0.29 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 15 | 0.29 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 4 | 0.29 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 4 | 0.29 |
| (1,3007) | 1:212:A:LYS:HB2 | 1:214:A:ALA:H | 8 | 0.29 |
| (1,3007) | 1:212:A:LYS:HB3 | 1:214:A:ALA:H | 8 | 0.29 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 15 | 0.29 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 15 | 0.29 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 15 | 0.29 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 18 | 0.29 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 18 | 0.29 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 18 | 0.29 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 15 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 2 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 2 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 2 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 12 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 12 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 12 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 20 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 20 | 0.29 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 20 | 0.29 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 14 | 0.29 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 6 | 0.29 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 10 | 0.29 |
| (1,2800) | 1:174:A:GLU:H | 1:174:A:GLU:HG3 | 12 | 0.29 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 7 | 0.29 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 9 | 0.29 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 13 | 0.29 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 6 | 0.29 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 11 | 0.29 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 1 | 0.29 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 9 | 0.29 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 9 | 0.29 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 9 | 0.29 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 15 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 15 | 0.29 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 15 | 0.29 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 20 | 0.29 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 20 | 0.29 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 20 | 0.29 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 16 | 0.29 |
| (1,2652) | 1:149:A:ALA:H | 1:179:A:LEU:HB3 | 19 | 0.29 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 18 | 0.29 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 2 | 0.29 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 13 | 0.29 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 13 | 0.29 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 1 | 0.29 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 1 | 0.29 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 1 | 0.29 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 9 | 0.29 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 10 | 0.29 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 16 | 0.29 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 16 | 0.29 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 3 | 0.29 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 17 | 0.29 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 14 | 0.29 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 14 | 0.29 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 14 | 0.29 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 14 | 0.29 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 13 | 0.29 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 13 | 0.29 |
| (1,2241) | 1:69:A:PHE:H | 1:86:A:GLU:HG2 | 7 | 0.29 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 1 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 19 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 19 | 0.29 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 19 | 0.29 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 14 | 0.29 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 6 | 0.29 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 6 | 0.29 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 6 | 0.29 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 15 | 0.29 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 15 | 0.29 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 15 | 0.29 |
| (1,2002) | 1:216:A:LEU:H | 1:216:A:LEU:HG | 3 | 0.29 |
| (1,1963) | 1:161:A:LYS:HD2 | 1:189:A:VAL:H | 16 | 0.29 |
| (1,1963) | 1:161:A:LYS:HD3 | 1:189:A:VAL:H | 16 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 5 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 5 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 5 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 12 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 12 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 12 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 19 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 19 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 19 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 20 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 20 | 0.29 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 20 | 0.29 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 11 | 0.29 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 11 | 0.29 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 11 | 0.29 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 16 | 0.29 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 16 | 0.29 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 16 | 0.29 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 6 | 0.29 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 6 | 0.29 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 20 | 0.29 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 20 | 0.29 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 12 | 0.29 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 13 | 0.29 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 13 | 0.29 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 13 | 0.29 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 4 | 0.29 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 18 | 0.29 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 16 | 0.29 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 16 | 0.29 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 16 | 0.29 |
| (1,1588) | 1:184:A:ILE:H | 1:185:A:LYS:HE3 | 2 | 0.29 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 10 | 0.29 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 10 | 0.29 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 10 | 0.29 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 14 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 3 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 3 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 3 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 14 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 14 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 14 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 17 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 17 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 17 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 19 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 19 | 0.29 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 19 | 0.29 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 15 | 0.29 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 6 | 0.29 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 6 | 0.29 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 6 | 0.29 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 20 | 0.29 |
| (1,1380) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB2 | 12 | 0.29 |
| (1,1380) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB2 | 12 | 0.29 |
| (1,1380) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB2 | 12 | 0.29 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 7 | 0.29 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 7 | 0.29 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 10 | 0.29 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 10 | 0.29 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE2 | 11 | 0.29 |
| (1,1361) | 1:201:A:ILE:HA | 1:205:A:LYS:HE3 | 11 | 0.29 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 19 | 0.29 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 15 | 0.29 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 15 | 0.29 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 15 | 0.29 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 15 | 0.29 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 13 | 0.29 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 13 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 13 | 0.29 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 5 | 0.29 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 5 | 0.29 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 5 | 0.29 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 3 | 0.29 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 13 | 0.29 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 17 | 0.29 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 17 | 0.29 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 17 | 0.29 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 6 | 0.29 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 6 | 0.29 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB1 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB2 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB3 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB1 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB2 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB3 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB1 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB2 | 20 | 0.29 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB3 | 20 | 0.29 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 3 | 0.29 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 3 | 0.29 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 6 | 0.29 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 7 | 0.29 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 7 | 0.29 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 7 | 0.29 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 7 | 0.29 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 7 | 0.29 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 7 | 0.29 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 7 | 0.29 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 7 | 0.29 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 7 | 0.29 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 9 | 0.29 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 9 | 0.29 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 9 | 0.29 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 9 | 0.29 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 9 | 0.29 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 9 | 0.29 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 8 | 0.29 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 8 | 0.29 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 8 | 0.29 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 7 | 0.29 |
| (1,864) | 1:191:A:THR:HA | 1:192:A:ILE:HG13 | 8 | 0.29 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 4 | 0.29 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 4 | 0.29 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 4 | 0.29 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 3 | 0.29 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 3 | 0.29 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 3 | 0.29 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 3 | 0.29 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 3 | 0.29 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 3 | 0.29 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 10 | 0.29 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 10 | 0.29 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 10 | 0.29 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 10 | 0.29 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 10 | 0.29 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 10 | 0.29 |
| (1,794) | 1:73:A:VAL:HG11 | 1:83:A:GLN:HG2 | 20 | 0.29 |
| (1,794) | 1:73:A:VAL:HG12 | 1:83:A:GLN:HG2 | 20 | 0.29 |
| (1,794) | 1:73:A:VAL:HG13 | 1:83:A:GLN:HG2 | 20 | 0.29 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 11 | 0.29 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 6 | 0.29 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 6 | 0.29 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 6 | 0.29 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 6 | 0.29 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 6 | 0.29 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 6 | 0.29 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 3 | 0.29 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 2 | 0.29 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG21 | 10 | 0.29 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG22 | 10 | 0.29 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG23 | 10 | 0.29 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 3 | 0.29 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 3 | 0.29 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 6 | 0.29 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 6 | 0.29 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 16 | 0.29 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 16 | 0.29 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 19 | 0.29 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 19 | 0.29 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 19 | 0.29 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 19 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 19 | 0.29 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 19 | 0.29 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD2 | 15 | 0.29 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD3 | 15 | 0.29 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 1 | 0.29 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 5 | 0.29 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 8 | 0.29 |
| (1,483) | 1:82:A:LEU:HG | 1:112:A:TYR:H | 6 | 0.29 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 1 | 0.29 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 1 | 0.29 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 4 | 0.29 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 4 | 0.29 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 19 | 0.29 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 19 | 0.29 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 19 | 0.29 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 12 | 0.29 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 12 | 0.29 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 12 | 0.29 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 16 | 0.29 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 16 | 0.29 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 16 | 0.29 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 2 | 0.29 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 2 | 0.29 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 2 | 0.29 |
| (1,261) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HZ | 10 | 0.29 |
| (1,261) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HZ | 10 | 0.29 |
| (1,261) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HZ | 10 | 0.29 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 9 | 0.29 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 4 | 0.29 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 4 | 0.29 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 4 | 0.29 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 7 | 0.29 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 7 | 0.29 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 7 | 0.29 |
| (1,81) | 1:52:A:VAL:HG11 | 1:53:A:THR:HB | 7 | 0.29 |
| (1,81) | 1:52:A:VAL:HG12 | 1:53:A:THR:HB | 7 | 0.29 |
| (1,81) | 1:52:A:VAL:HG13 | 1:53:A:THR:HB | 7 | 0.29 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 8 | 0.29 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 12 | 0.28 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 12 | 0.28 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD2 | 10 | 0.28 |
| (1,3999) | 2:4:B:LYS:HD2 | 2:5:B:PRO:HD3 | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD2 | 10 | 0.28 |
| (1,3999) | 2:4:B:LYS:HD3 | 2:5:B:PRO:HD3 | 10 | 0.28 |
| (1,3990) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 14 | 0.28 |
| (1,3990) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 14 | 0.28 |
| (1,3990) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 14 | 0.28 |
| (1,3990) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 14 | 0.28 |
| (1,3990) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 14 | 0.28 |
| (1,3990) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 14 | 0.28 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 11 | 0.28 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 11 | 0.28 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 11 | 0.28 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 11 | 0.28 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 11 | 0.28 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 11 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 8 | 0.28 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 8 | 0.28 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 17 | 0.28 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 17 | 0.28 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 17 | 0.28 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 17 | 0.28 |
| (1,3643) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 2 | 0.28 |
| (1,3643) | 1:85:A:ASP:HB3 | 1:108:A:GLY:HA2 | 2 | 0.28 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB2 | 8 | 0.28 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 8 | 0.28 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB2 | 8 | 0.28 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 8 | 0.28 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB2 | 8 | 0.28 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 8 | 0.28 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 13 | 0.28 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 11 | 0.28 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 15 | 0.28 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 9 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 9 | 0.28 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 12 | 0.28 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 12 | 0.28 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 12 | 0.28 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 9 | 0.28 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 9 | 0.28 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 9 | 0.28 |
| (1,3430) | 2:9:B:ILE:HA | 2:20:B:ARG:HG2 | 12 | 0.28 |
| (1,3430) | 2:9:B:ILE:HA | 2:20:B:ARG:HG3 | 12 | 0.28 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 19 | 0.28 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 19 | 0.28 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 19 | 0.28 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 11 | 0.28 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 11 | 0.28 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 12 | 0.28 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 12 | 0.28 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 4 | 0.28 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 4 | 0.28 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 4 | 0.28 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 3 | 0.28 |
| (1,3329) | 2:20:B:ARG:HD2 | 2:21:B:MET:H | 18 | 0.28 |
| (1,3329) | 2:20:B:ARG:HD3 | 2:21:B:MET:H | 18 | 0.28 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 10 | 0.28 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 2 | 0.28 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 11 | 0.28 |
| (1,3294) | 2:8:B:ILE:HD11 | 2:21:B:MET:HG2 | 2 | 0.28 |
| (1,3294) | 2:8:B:ILE:HD12 | 2:21:B:MET:HG2 | 2 | 0.28 |
| (1,3294) | 2:8:B:ILE:HD13 | 2:21:B:MET:HG2 | 2 | 0.28 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 6 | 0.28 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 6 | 0.28 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 16 | 0.28 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 16 | 0.28 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 16 | 0.28 |
| (1,3208) | 1:126:A:ALA:HB1 | 1:133:A:TRP:HD1 | 18 | 0.28 |
| (1,3208) | 1:126:A:ALA:HB2 | 1:133:A:TRP:HD1 | 18 | 0.28 |
| (1,3208) | 1:126:A:ALA:HB3 | 1:133:A:TRP:HD1 | 18 | 0.28 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 20 | 0.28 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 13 | 0.28 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 13 | 0.28 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 13 | 0.28 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 13 | 0.28 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 13 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 13 | 0.28 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 10 | 0.28 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 10 | 0.28 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 17 | 0.28 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 12 | 0.28 |
| (1,3068) | 1:195:A:ASN:HA | 1:196:A:ASN:HD21 | 14 | 0.28 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 2 | 0.28 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 1 | 0.28 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 19 | 0.28 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 19 | 0.28 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 19 | 0.28 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 14 | 0.28 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 14 | 0.28 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 14 | 0.28 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 12 | 0.28 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 12 | 0.28 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 12 | 0.28 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 19 | 0.28 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 19 | 0.28 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 19 | 0.28 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 18 | 0.28 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 2 | 0.28 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 7 | 0.28 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 10 | 0.28 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 17 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 2 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 4 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 8 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 11 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 13 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 14 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 15 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 16 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 17 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 18 | 0.28 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 20 | 0.28 |
| (1,2800) | 1:174:A:GLU:H | 1:174:A:GLU:HG3 | 1 | 0.28 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB1 | 1 | 0.28 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB2 | 1 | 0.28 |
| (1,2780) | 1:170:A:PHE:H | 1:176:A:ALA:HB3 | 1 | 0.28 |
| (1,2765) | 1:168:A:ALA:H | 1:196:A:ASN:HA | 5 | 0.28 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 9 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2761) | 1:167:A:ASP:H | 1:196:A:ASN:HB2 | 13 | 0.28 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 18 | 0.28 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 18 | 0.28 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 18 | 0.28 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 10 | 0.28 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 8 | 0.28 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 9 | 0.28 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 14 | 0.28 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 14 | 0.28 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 14 | 0.28 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 18 | 0.28 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 18 | 0.28 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 18 | 0.28 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 14 | 0.28 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 14 | 0.28 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 14 | 0.28 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 16 | 0.28 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 6 | 0.28 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 1 | 0.28 |
| (1,2543) | 1:130:A:THR:HG21 | 1:131:A:LYS:H | 20 | 0.28 |
| (1,2543) | 1:130:A:THR:HG22 | 1:131:A:LYS:H | 20 | 0.28 |
| (1,2543) | 1:130:A:THR:HG23 | 1:131:A:LYS:H | 20 | 0.28 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 9 | 0.28 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 11 | 0.28 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 13 | 0.28 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 8 | 0.28 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 8 | 0.28 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 8 | 0.28 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 12 | 0.28 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD1 | 1 | 0.28 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD2 | 1 | 0.28 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 3 | 0.28 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 13 | 0.28 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 8 | 0.28 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 8 | 0.28 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 8 | 0.28 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 1 | 0.28 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 1 | 0.28 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 1 | 0.28 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 15 | 0.28 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 15 | 0.28 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 18 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 2 | 0.28 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 2 | 0.28 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 6 | 0.28 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 12 | 0.28 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 12 | 0.28 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 12 | 0.28 |
| (1,2002) | 1:216:A:LEU:H | 1:216:A:LEU:HG | 12 | 0.28 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 5 | 0.28 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 20 | 0.28 |
| (1,1997) | 1:184:A:ILE:HA | 1:216:A:LEU:HB3 | 1 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 12 | 0.28 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 12 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 2 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 2 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 2 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 7 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 7 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 7 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 10 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 10 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 10 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 14 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 14 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 14 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 15 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 15 | 0.28 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 8 | 0.28 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 8 | 0.28 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 8 | 0.28 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 4 | 0.28 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 4 | 0.28 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 14 | 0.28 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 14 | 0.28 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 14 | 0.28 |
| (1,1731) | 1:167:A:ASP:HA | 1:196:A:ASN:HB3 | 13 | 0.28 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 2 | 0.28 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 7 | 0.28 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD11 | 9 | 0.28 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD12 | 9 | 0.28 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD13 | 9 | 0.28 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 20 | 0.28 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 5 | 0.28 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 5 | 0.28 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 5 | 0.28 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 7 | 0.28 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 8 | 0.28 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 13 | 0.28 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 16 | 0.28 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 16 | 0.28 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 16 | 0.28 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 1 | 0.28 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 1 | 0.28 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 1 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 1 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 1 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 1 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 4 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 4 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 4 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 19 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 19 | 0.28 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 19 | 0.28 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 15 | 0.28 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 17 | 0.28 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 17 | 0.28 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 17 | 0.28 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 9 | 0.28 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 9 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 9 | 0.28 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 12 | 0.28 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 12 | 0.28 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 12 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 12 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 12 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 12 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 12 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 12 | 0.28 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 12 | 0.28 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 5 | 0.28 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 6 | 0.28 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 6 | 0.28 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 6 | 0.28 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 9 | 0.28 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 9 | 0.28 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 9 | 0.28 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 16 | 0.28 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 12 | 0.28 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 12 | 0.28 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 12 | 0.28 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 20 | 0.28 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 19 | 0.28 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 1 | 0.28 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 1 | 0.28 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG21 | 1 | 0.28 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG22 | 1 | 0.28 |
| (1,1330) | 1:157:A:LEU:HG | 1:162:A:THR:HG23 | 1 | 0.28 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 1 | 0.28 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 18 | 0.28 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 2 | 0.28 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 2 | 0.28 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 11 | 0.28 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 4 | 0.28 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 4 | 0.28 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 4 | 0.28 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 10 | 0.28 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 10 | 0.28 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 10 | 0.28 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 8 | 0.28 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 8 | 0.28 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 8 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 9 | 0.28 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 9 | 0.28 |
| (1,1135) | 1:145:A:ALA:HB1 | 1:146:A:PRO:HG2 | 12 | 0.28 |
| (1,1135) | 1:145:A:ALA:HB2 | 1:146:A:PRO:HG2 | 12 | 0.28 |
| (1,1135) | 1:145:A:ALA:HB3 | 1:146:A:PRO:HG2 | 12 | 0.28 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 17 | 0.28 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 17 | 0.28 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 17 | 0.28 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 15 | 0.28 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 14 | 0.28 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 14 | 0.28 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 6 | 0.28 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 6 | 0.28 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 6 | 0.28 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 20 | 0.28 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 20 | 0.28 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 20 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 2 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 2 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 2 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 15 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 15 | 0.28 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 15 | 0.28 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 19 | 0.28 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 11 | 0.28 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 11 | 0.28 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 6 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 6 | 0.28 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 6 | 0.28 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 17 | 0.28 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 17 | 0.28 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 9 | 0.28 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 10 | 0.28 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 10 | 0.28 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 10 | 0.28 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 10 | 0.28 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 10 | 0.28 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 10 | 0.28 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 11 | 0.28 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 11 | 0.28 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 11 | 0.28 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 11 | 0.28 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 11 | 0.28 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 11 | 0.28 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 5 | 0.28 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 5 | 0.28 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 5 | 0.28 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 2 | 0.28 |
| (1,796) | 1:116:A:GLN:HG3 | 1:187:A:MET:HA | 2 | 0.28 |
| (1,729) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 2 | 0.28 |
| (1,729) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 13 | 0.28 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG21 | 11 | 0.28 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG22 | 11 | 0.28 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG23 | 11 | 0.28 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD21 | 15 | 0.28 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD22 | 15 | 0.28 |
| (1,612) | 1:181:A:GLU:HB2 | 1:216:A:LEU:HD23 | 15 | 0.28 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD21 | 15 | 0.28 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD22 | 15 | 0.28 |
| (1,612) | 1:181:A:GLU:HB3 | 1:216:A:LEU:HD23 | 15 | 0.28 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 3 | 0.28 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 7 | 0.28 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 3 | 0.28 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 3 | 0.28 |
| (1,446) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA3 | 18 | 0.28 |
| (1,446) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA3 | 18 | 0.28 |
| (1,446) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA3 | 18 | 0.28 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 16 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 16 | 0.28 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 16 | 0.28 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 7 | 0.28 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 7 | 0.28 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 7 | 0.28 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 18 | 0.28 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 18 | 0.28 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 18 | 0.28 |
| (1,330) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HA | 5 | 0.28 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 1 | 0.28 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 1 | 0.28 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 1 | 0.28 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 12 | 0.28 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 12 | 0.28 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 12 | 0.28 |
| (1,281) | 1:68:A:VAL:HG11 | 1:86:A:GLU:HG2 | 17 | 0.28 |
| (1,281) | 1:68:A:VAL:HG12 | 1:86:A:GLU:HG2 | 17 | 0.28 |
| (1,281) | 1:68:A:VAL:HG13 | 1:86:A:GLU:HG2 | 17 | 0.28 |
| (1,281) | 1:68:A:VAL:HG21 | 1:86:A:GLU:HG2 | 17 | 0.28 |
| (1,281) | 1:68:A:VAL:HG22 | 1:86:A:GLU:HG2 | 17 | 0.28 |
| (1,281) | 1:68:A:VAL:HG23 | 1:86:A:GLU:HG2 | 17 | 0.28 |
| (1,183) | 1:58:A:HIS:HB3 | 2:12:B:ASN:HD22 | 12 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 11 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 11 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 11 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 14 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 14 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 14 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 18 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 18 | 0.28 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 18 | 0.28 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 4 | 0.28 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 15 | 0.28 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 3 | 0.28 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 3 | 0.28 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 3 | 0.28 |
| (1,33) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB3 | 19 | 0.28 |
| (1,33) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB3 | 19 | 0.28 |
| (1,33) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB3 | 19 | 0.28 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 17 | 0.28 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 19 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 19 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 19 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 19 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 19 | 0.27 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 19 | 0.27 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 13 | 0.27 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 13 | 0.27 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 13 | 0.27 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 13 | 0.27 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 13 | 0.27 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 13 | 0.27 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 8 | 0.27 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 8 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 6 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 6 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 6 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 6 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 6 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 6 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 18 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 18 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 18 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 18 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 18 | 0.27 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 18 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 3 | 0.27 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 3 | 0.27 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD21 | 4 | 0.27 |
| (1,3552) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HD22 | 4 | 0.27 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD21 | 4 | 0.27 |
| (1,3552) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HD22 | 4 | 0.27 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD21 | 4 | 0.27 |
| (1,3552) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HD22 | 4 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3515) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HB | 6 | 0.27 |
| (1,3515) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HB | 6 | 0.27 |
| (1,3511) | 1:51:A:PRO:HB2 | 2:9:B:ILE:HG12 | 3 | 0.27 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 16 | 0.27 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 9 | 0.27 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 9 | 0.27 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 9 | 0.27 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 9 | 0.27 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 9 | 0.27 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 9 | 0.27 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 12 | 0.27 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 12 | 0.27 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 12 | 0.27 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 11 | 0.27 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 11 | 0.27 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 11 | 0.27 |
| (1,3433) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD2 | 3 | 0.27 |
| (1,3433) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD3 | 3 | 0.27 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 8 | 0.27 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 8 | 0.27 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 8 | 0.27 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 10 | 0.27 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 10 | 0.27 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 5 | 0.27 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 5 | 0.27 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 5 | 0.27 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 13 | 0.27 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 14 | 0.27 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 18 | 0.27 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 14 | 0.27 |
| (1,3237) | 1:90:A:HIS:H | 1:90:A:HIS:HE1 | 19 | 0.27 |
| (1,3229) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD21 | 10 | 0.27 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 14 | 0.27 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 14 | 0.27 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 1 | 0.27 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 1 | 0.27 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 1 | 0.27 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 1 | 0.27 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 1 | 0.27 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 1 | 0.27 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG11 | 17 | 0.27 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG12 | 17 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG13 | 17 | 0.27 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG11 | 17 | 0.27 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG12 | 17 | 0.27 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG13 | 17 | 0.27 |
| (1,3126) | 1:112:A:TYR:HE1 | 1:114:A:ASP:H | 4 | 0.27 |
| (1,3126) | 1:112:A:TYR:HE2 | 1:114:A:ASP:H | 4 | 0.27 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 15 | 0.27 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 5 | 0.27 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 20 | 0.27 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 9 | 0.27 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 16 | 0.27 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 16 | 0.27 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 16 | 0.27 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 18 | 0.27 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 18 | 0.27 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 18 | 0.27 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 6 | 0.27 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 6 | 0.27 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 6 | 0.27 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 10 | 0.27 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 10 | 0.27 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 10 | 0.27 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 2 | 0.27 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 2 | 0.27 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 2 | 0.27 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 2 | 0.27 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 4 | 0.27 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 15 | 0.27 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 10 | 0.27 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 10 | 0.27 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 10 | 0.27 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 18 | 0.27 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 18 | 0.27 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 18 | 0.27 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 8 | 0.27 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 3 | 0.27 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 5 | 0.27 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 9 | 0.27 |
| (1,2801) | 1:174:A:GLU:H | 1:174:A:GLU:HB3 | 19 | 0.27 |
| (1,2800) | 1:174:A:GLU:H | 1:174:A:GLU:HG3 | 7 | 0.27 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 2 | 0.27 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 9 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2765) | 1:168:A:ALA:H | 1:196:A:ASN:HA | 4 | 0.27 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 3 | 0.27 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 18 | 0.27 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 14 | 0.27 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 14 | 0.27 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 14 | 0.27 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 3 | 0.27 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 7 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 1 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 1 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 1 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 3 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 3 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 3 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 9 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 9 | 0.27 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 9 | 0.27 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 9 | 0.27 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 9 | 0.27 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 9 | 0.27 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 2 | 0.27 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 3 | 0.27 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 7 | 0.27 |
| (1,2393) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 18 | 0.27 |
| (1,2383) | 1:100:A:PRO:HB3 | 1:101:A:VAL:H | 15 | 0.27 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 3 | 0.27 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 6 | 0.27 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 18 | 0.27 |
| (1,2120) | 1:74:A:ASP:HA | 1:83:A:GLN:HG3 | 17 | 0.27 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 3 | 0.27 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 3 | 0.27 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 3 | 0.27 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 20 | 0.27 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 20 | 0.27 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 20 | 0.27 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 10 | 0.27 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 10 | 0.27 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 10 | 0.27 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 1 | 0.27 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 4 | 0.27 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 11 | 0.27 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD21 | 13 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD22 | 13 | 0.27 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD23 | 13 | 0.27 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 20 | 0.27 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD2 | 13 | 0.27 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD3 | 13 | 0.27 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD2 | 13 | 0.27 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD3 | 13 | 0.27 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD2 | 13 | 0.27 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD3 | 13 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG21 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG22 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD11 | 1:219:A:THR:HG23 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG21 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG22 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD12 | 1:219:A:THR:HG23 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG21 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG22 | 5 | 0.27 |
| (1,2024) | 1:192:A:ILE:HD13 | 1:219:A:THR:HG23 | 5 | 0.27 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 19 | 0.27 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 19 | 0.27 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 19 | 0.27 |
| (1,2002) | 1:216:A:LEU:H | 1:216:A:LEU:HG | 15 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 6 | 0.27 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 6 | 0.27 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 9 | 0.27 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 9 | 0.27 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 9 | 0.27 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 6 | 0.27 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 6 | 0.27 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 6 | 0.27 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 7 | 0.27 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 7 | 0.27 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 7 | 0.27 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 7 | 0.27 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 11 | 0.27 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 11 | 0.27 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 3 | 0.27 |
| (1,1815) | 1:201:A:ILE:HG21 | 1:205:A:LYS:H | 3 | 0.27 |
| (1,1815) | 1:201:A:ILE:HG22 | 1:205:A:LYS:H | 3 | 0.27 |
| (1,1815) | 1:201:A:ILE:HG23 | 1:205:A:LYS:H | 3 | 0.27 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 13 | 0.27 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 3 | 0.27 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 8 | 0.27 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 3 | 0.27 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 9 | 0.27 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 6 | 0.27 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 6 | 0.27 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 6 | 0.27 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 16 | 0.27 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 16 | 0.27 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 16 | 0.27 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 3 | 0.27 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 11 | 0.27 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 14 | 0.27 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 15 | 0.27 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 17 | 0.27 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 5 | 0.27 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 5 | 0.27 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 5 | 0.27 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE2 | 18 | 0.27 |
| (1,1589) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HE3 | 18 | 0.27 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 1 | 0.27 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 4 | 0.27 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 8 | 0.27 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 8 | 0.27 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 8 | 0.27 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 10 | 0.27 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 20 | 0.27 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 20 | 0.27 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 20 | 0.27 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 19 | 0.27 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 19 | 0.27 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 19 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 5 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 5 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 5 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 5 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 5 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 5 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 7 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 7 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 7 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 7 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 7 | 0.27 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 7 | 0.27 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 10 | 0.27 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 7 | 0.27 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 10 | 0.27 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 4 | 0.27 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 13 | 0.27 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 6 | 0.27 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 8 | 0.27 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 11 | 0.27 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 10 | 0.27 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 17 | 0.27 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 17 | 0.27 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 16 | 0.27 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 16 | 0.27 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 16 | 0.27 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG21 | 1 | 0.27 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG22 | 1 | 0.27 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG23 | 1 | 0.27 |
| (1,1321) | 1:158:A:ASP:HB2 | 1:162:A:THR:HA | 16 | 0.27 |
| (1,1284) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 17 | 0.27 |
| (1,1284) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 17 | 0.27 |
| (1,1284) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 17 | 0.27 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 10 | 0.27 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 10 | 0.27 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 10 | 0.27 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 4 | 0.27 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 4 | 0.27 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 4 | 0.27 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 9 | 0.27 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 9 | 0.27 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 9 | 0.27 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 3 | 0.27 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 3 | 0.27 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 7 | 0.27 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 11 | 0.27 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 11 | 0.27 |
| (1,1150) | 1:148:A:SER:HA | 1:179:A:LEU:HB3 | 19 | 0.27 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB1 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB2 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB3 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB1 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB2 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB3 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB1 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB2 | 7 | 0.27 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB3 | 7 | 0.27 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 10 | 0.27 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 13 | 0.27 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 20 | 0.27 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 20 | 0.27 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 20 | 0.27 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 20 | 0.27 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 20 | 0.27 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 20 | 0.27 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 8 | 0.27 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 8 | 0.27 |
| (1,1105) | 1:141:A:GLU:HG2 | 1:142:A:THR:HB | 7 | 0.27 |
| (1,1105) | 1:141:A:GLU:HG3 | 1:142:A:THR:HB | 7 | 0.27 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 12 | 0.27 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 12 | 0.27 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 12 | 0.27 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 12 | 0.27 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 12 | 0.27 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 12 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 10 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 10 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 10 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 17 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 17 | 0.27 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 17 | 0.27 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 5 | 0.27 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 11 | 0.27 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 13 | 0.27 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 13 | 0.27 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 11 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 11 | 0.27 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 11 | 0.27 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 9 | 0.27 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 9 | 0.27 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD21 | 11 | 0.27 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD22 | 11 | 0.27 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD23 | 11 | 0.27 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 8 | 0.27 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 8 | 0.27 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 8 | 0.27 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 14 | 0.27 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 14 | 0.27 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 14 | 0.27 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 14 | 0.27 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 14 | 0.27 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 14 | 0.27 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 18 | 0.27 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 18 | 0.27 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 18 | 0.27 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 20 | 0.27 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 20 | 0.27 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 20 | 0.27 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 3 | 0.27 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 3 | 0.27 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 3 | 0.27 |
| (1,813) | 1:117:A:VAL:HG21 | 1:187:A:MET:HG3 | 12 | 0.27 |
| (1,813) | 1:117:A:VAL:HG22 | 1:187:A:MET:HG3 | 12 | 0.27 |
| (1,813) | 1:117:A:VAL:HG23 | 1:187:A:MET:HG3 | 12 | 0.27 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 7 | 0.27 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 10 | 0.27 |
| (1,776) | 1:113:A:ASP:HA | 1:118:A:ILE:HG12 | 10 | 0.27 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 3 | 0.27 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 15 | 0.27 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 4 | 0.27 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB2 | 9 | 0.27 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB3 | 9 | 0.27 |
| (1,676) | 1:103:A:THR:HG21 | 1:128:A:LEU:H | 13 | 0.27 |
| (1,676) | 1:103:A:THR:HG22 | 1:128:A:LEU:H | 13 | 0.27 |
| (1,676) | 1:103:A:THR:HG23 | 1:128:A:LEU:H | 13 | 0.27 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 1 | 0.27 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 1 | 0.27 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 18 | 0.27 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 18 | 0.27 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 20 | 0.27 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 18 | 0.27 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 18 | 0.27 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 18 | 0.27 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 13 | 0.27 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 13 | 0.27 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 13 | 0.27 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 1 | 0.27 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 1 | 0.27 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 1 | 0.27 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 19 | 0.27 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 19 | 0.27 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 19 | 0.27 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 8 | 0.27 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 20 | 0.27 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 15 | 0.27 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 15 | 0.27 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 15 | 0.27 |
| (1,277) | 1:155:A:LYS:HE2 | 1:164:A:GLU:HB2 | 13 | 0.27 |
| (1,277) | 1:155:A:LYS:HE2 | 1:164:A:GLU:HB3 | 13 | 0.27 |
| (1,232) | 1:64:A:PRO:HA | 1:91:A:GLN:HE22 | 2 | 0.27 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 18 | 0.27 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 18 | 0.27 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 18 | 0.27 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 5 | 0.27 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 3 | 0.27 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 3 | 0.27 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 3 | 0.27 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 14 | 0.27 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 14 | 0.27 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 14 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 13 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 13 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 13 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 14 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 14 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 14 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 15 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 15 | 0.27 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 15 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 5 | 0.27 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 5 | 0.27 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 5 | 0.27 |
| (1,21) | 1:47:A:THR:HG21 | 1:51:A:PRO:HD2 | 15 | 0.27 |
| (1,21) | 1:47:A:THR:HG22 | 1:51:A:PRO:HD2 | 15 | 0.27 |
| (1,21) | 1:47:A:THR:HG23 | 1:51:A:PRO:HD2 | 15 | 0.27 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 11 | 0.27 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 11 | 0.27 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 11 | 0.27 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 2 | 0.26 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 2 | 0.26 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 15 | 0.26 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 15 | 0.26 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 15 | 0.26 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 15 | 0.26 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 15 | 0.26 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 15 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 9 | 0.26 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 9 | 0.26 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 17 | 0.26 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 17 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE1 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD11 | 1:165:A:PHE:HE2 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE1 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD12 | 1:165:A:PHE:HE2 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE1 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD13 | 1:165:A:PHE:HE2 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE1 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD21 | 1:165:A:PHE:HE2 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE1 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD22 | 1:165:A:PHE:HE2 | 10 | 0.26 |
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE1 | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3810) | 1:119:A:LEU:HD23 | 1:165:A:PHE:HE2 | 10 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 4 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 8 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 8 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 11 | 0.26 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 11 | 0.26 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 8 | 0.26 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 8 | 0.26 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 14 | 0.26 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 14 | 0.26 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 8 | 0.26 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 8 | 0.26 |
| (1,3643) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 13 | 0.26 |
| (1,3643) | 1:85:A:ASP:HB3 | 1:108:A:GLY:HA2 | 13 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 10 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 10 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 10 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 10 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 10 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 10 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 16 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 16 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 16 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 16 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 16 | 0.26 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 16 | 0.26 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 1 | 0.26 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 1 | 0.26 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 1 | 0.26 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD2 | 20 | 0.26 |
| (1,3514) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HD3 | 20 | 0.26 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 12 | 0.26 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 12 | 0.26 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 12 | 0.26 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 12 | 0.26 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 12 | 0.26 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HD11 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HD12 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HD13 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HD11 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HD12 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HD13 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HD11 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HD12 | 12 | 0.26 |
| (1,3484) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HD13 | 12 | 0.26 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 4 | 0.26 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 4 | 0.26 |
| (1,3474) | 2:17:B:LYS:HD2 | 2:18:B:CYS:H | 13 | 0.26 |
| (1,3474) | 2:17:B:LYS:HD3 | 2:18:B:CYS:H | 13 | 0.26 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 11 | 0.26 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 11 | 0.26 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 11 | 0.26 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 17 | 0.26 |
| (1,3368) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 17 | 0.26 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 17 | 0.26 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 17 | 0.26 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 6 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 20 | 0.26 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 20 | 0.26 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 20 | 0.26 |
| (1,3284) | 1:68:A:VAL:HA | 1:69:A:PHE:HZ | 2 | 0.26 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 11 | 0.26 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 11 | 0.26 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 11 | 0.26 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 2 | 0.26 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 13 | 0.26 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 16 | 0.26 |
| (1,3248) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HE1 | 18 | 0.26 |
| (1,3248) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HE1 | 18 | 0.26 |
| (1,3248) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HE1 | 18 | 0.26 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 6 | 0.26 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 17 | 0.26 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 4 | 0.26 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 3 | 0.26 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 3 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 1 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 1 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 1 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 1 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 1 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 1 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 16 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 16 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 16 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 16 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 16 | 0.26 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 16 | 0.26 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 4 | 0.26 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 4 | 0.26 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 4 | 0.26 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 4 | 0.26 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 4 | 0.26 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 4 | 0.26 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 6 | 0.26 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 6 | 0.26 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 7 | 0.26 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 7 | 0.26 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 3 | 0.26 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3062) | 1:85:A:ASP:H | 1:109:A:ASN:HD21 | 9 | 0.26 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 12 | 0.26 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 4 | 0.26 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 8 | 0.26 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 15 | 0.26 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 15 | 0.26 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 15 | 0.26 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 20 | 0.26 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 20 | 0.26 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 20 | 0.26 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 4 | 0.26 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 17 | 0.26 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 2 | 0.26 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 7 | 0.26 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 13 | 0.26 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 15 | 0.26 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 19 | 0.26 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 15 | 0.26 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 15 | 0.26 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 15 | 0.26 |
| (1,2634) | 1:142:A:THR:HB | 1:147:A:GLY:H | 12 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 17 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 17 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 17 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 20 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 20 | 0.26 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 20 | 0.26 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 5 | 0.26 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 5 | 0.26 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 5 | 0.26 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 8 | 0.26 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 8 | 0.26 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 8 | 0.26 |
| (1,2617) | 1:117:A:VAL:HB | 1:143:A:VAL:H | 18 | 0.26 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 5 | 0.26 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 5 | 0.26 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 5 | 0.26 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 12 | 0.26 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 16 | 0.26 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 16 | 0.26 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 16 | 0.26 |
| (1,2497) | 1:121:A:GLY:H | 1:138:A:ALA:HB1 | 19 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2497) | 1:121:A:GLY:H | 1:138:A:ALA:HB2 | 19 | 0.26 |
| (1,2497) | 1:121:A:GLY:H | 1:138:A:ALA:HB3 | 19 | 0.26 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 14 | 0.26 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD11 | 19 | 0.26 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD12 | 19 | 0.26 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD13 | 19 | 0.26 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 1 | 0.26 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 12 | 0.26 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 12 | 0.26 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 20 | 0.26 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 20 | 0.26 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 20 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 12 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 16 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 18 | 0.26 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 18 | 0.26 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 12 | 0.26 |
| (1,2091) | 1:123:A:LYS:HG2 | 1:136:A:TYR:HB3 | 13 | 0.26 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 4 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 4 | 0.26 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 4 | 0.26 |
| (1,2016) | 1:190:A:LYS:HG3 | 1:218:A:ALA:HA | 9 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 14 | 0.26 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 14 | 0.26 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 3 | 0.26 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 3 | 0.26 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 3 | 0.26 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD21 | 17 | 0.26 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD22 | 17 | 0.26 |
| (1,1923) | 1:208:A:LYS:H | 1:209:A:LEU:HD23 | 17 | 0.26 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 8 | 0.26 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 8 | 0.26 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 8 | 0.26 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 6 | 0.26 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 6 | 0.26 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 6 | 0.26 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 1 | 0.26 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 1 | 0.26 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 13 | 0.26 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 13 | 0.26 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD2 | 12 | 0.26 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD3 | 12 | 0.26 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD2 | 12 | 0.26 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD3 | 12 | 0.26 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD2 | 12 | 0.26 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD3 | 12 | 0.26 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 6 | 0.26 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 4 | 0.26 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 4 | 0.26 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 4 | 0.26 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 5 | 0.26 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 12 | 0.26 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 15 | 0.26 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 18 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 20 | 0.26 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 17 | 0.26 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 17 | 0.26 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 17 | 0.26 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 17 | 0.26 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 19 | 0.26 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 12 | 0.26 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 19 | 0.26 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 19 | 0.26 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 19 | 0.26 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 9 | 0.26 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 9 | 0.26 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 9 | 0.26 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 16 | 0.26 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 3 | 0.26 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 16 | 0.26 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 12 | 0.26 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 12 | 0.26 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 12 | 0.26 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 20 | 0.26 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 20 | 0.26 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 20 | 0.26 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 20 | 0.26 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 20 | 0.26 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 20 | 0.26 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 8 | 0.26 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 8 | 0.26 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 8 | 0.26 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 9 | 0.26 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 9 | 0.26 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 9 | 0.26 |
| (1,1600) | 1:186:A:THR:HB | 1:187:A:MET:HG2 | 15 | 0.26 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 7 | 0.26 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 7 | 0.26 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 7 | 0.26 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 10 | 0.26 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 10 | 0.26 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 10 | 0.26 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 17 | 0.26 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 17 | 0.26 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 17 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 2 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 2 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 2 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 2 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 2 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 4 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 4 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 4 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 4 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 4 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 4 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 13 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 13 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 13 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 13 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 13 | 0.26 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 13 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 1 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 1 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 1 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 2 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 2 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 2 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 8 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 8 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 8 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 10 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 10 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 10 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 13 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 13 | 0.26 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 13 | 0.26 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 18 | 0.26 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 20 | 0.26 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 15 | 0.26 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 18 | 0.26 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 1 | 0.26 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 14 | 0.26 |
| (1,1363) | 1:153:A:VAL:H | 1:166:A:ASP:HB2 | 17 | 0.26 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 11 | 0.26 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 11 | 0.26 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 16 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 16 | 0.26 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 17 | 0.26 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 17 | 0.26 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 17 | 0.26 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 17 | 0.26 |
| (1,1320) | 1:162:A:THR:HA | 1:190:A:LYS:HB2 | 9 | 0.26 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 11 | 0.26 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 11 | 0.26 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 11 | 0.26 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 9 | 0.26 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 9 | 0.26 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 9 | 0.26 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 10 | 0.26 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 13 | 0.26 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 13 | 0.26 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 13 | 0.26 |
| (1,1120) | 1:142:A:THR:HG21 | 1:179:A:LEU:H | 19 | 0.26 |
| (1,1120) | 1:142:A:THR:HG22 | 1:179:A:LEU:H | 19 | 0.26 |
| (1,1120) | 1:142:A:THR:HG23 | 1:179:A:LEU:H | 19 | 0.26 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 20 | 0.26 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 3 | 0.26 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 3 | 0.26 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 3 | 0.26 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 3 | 0.26 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 3 | 0.26 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 3 | 0.26 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 11 | 0.26 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 11 | 0.26 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 11 | 0.26 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 11 | 0.26 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 11 | 0.26 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 11 | 0.26 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 1 | 0.26 |
| (1,1053) | 1:139:A:SER:HB3 | 1:140:A:ILE:H | 16 | 0.26 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 1 | 0.26 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 2 | 0.26 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 9 | 0.26 |
| (1,945) | 1:77:A:GLN:HG2 | 1:128:A:LEU:HD11 | 10 | 0.26 |
| (1,945) | 1:77:A:GLN:HG2 | 1:128:A:LEU:HD12 | 10 | 0.26 |
| (1,945) | 1:77:A:GLN:HG2 | 1:128:A:LEU:HD13 | 10 | 0.26 |
| (1,945) | 1:77:A:GLN:HG2 | 1:128:A:LEU:HD21 | 10 | 0.26 |
| (1,945) | 1:77:A:GLN:HG2 | 1:128:A:LEU:HD22 | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,945) | 1:77:A:GLN:HG2 | 1:128:A:LEU:HD23 | 10 | 0.26 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 3 | 0.26 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 11 | 0.26 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 16 | 0.26 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 8 | 0.26 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 8 | 0.26 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 8 | 0.26 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 15 | 0.26 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 15 | 0.26 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 16 | 0.26 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 16 | 0.26 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 16 | 0.26 |
| (1,591) | 1:93:A:GLU:HB2 | 1:94:A:ALA:H | 11 | 0.26 |
| (1,564) | 1:74:A:ASP:HA | 1:75:A:ILE:HB | 18 | 0.26 |
| (1,537) | 1:68:A:VAL:HG11 | 1:88:A:GLN:HG2 | 5 | 0.26 |
| (1,537) | 1:68:A:VAL:HG12 | 1:88:A:GLN:HG2 | 5 | 0.26 |
| (1,537) | 1:68:A:VAL:HG13 | 1:88:A:GLN:HG2 | 5 | 0.26 |
| (1,537) | 1:68:A:VAL:HG21 | 1:88:A:GLN:HG2 | 5 | 0.26 |
| (1,537) | 1:68:A:VAL:HG22 | 1:88:A:GLN:HG2 | 5 | 0.26 |
| (1,537) | 1:68:A:VAL:HG23 | 1:88:A:GLN:HG2 | 5 | 0.26 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 11 | 0.26 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 11 | 0.26 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 11 | 0.26 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 20 | 0.26 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 20 | 0.26 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 20 | 0.26 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 12 | 0.26 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 12 | 0.26 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 12 | 0.26 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 17 | 0.26 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 17 | 0.26 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 17 | 0.26 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 1 | 0.26 |
| (1,348) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HB2 | 20 | 0.26 |
| (1,348) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HB2 | 20 | 0.26 |
| (1,348) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HB2 | 20 | 0.26 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 17 | 0.26 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 17 | 0.26 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 17 | 0.26 |
| (1,196) | 1:167:A:ASP:HA | 1:196:A:ASN:HB2 | 4 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 1 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 1 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 1 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 5 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 5 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 5 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 12 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 12 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 12 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 17 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 17 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 17 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 20 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 20 | 0.26 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 20 | 0.26 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 4 | 0.26 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 4 | 0.26 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 4 | 0.26 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 9 | 0.26 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 9 | 0.26 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 9 | 0.26 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG21 | 15 | 0.26 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG22 | 15 | 0.26 |
| (1,175) | 1:58:A:HIS:HA | 1:70:A:THR:HG23 | 15 | 0.26 |
| (1,170) | 1:56:A:ALA:HB1 | 1:69:A:PHE:H | 10 | 0.26 |
| (1,170) | 1:56:A:ALA:HB2 | 1:69:A:PHE:H | 10 | 0.26 |
| (1,170) | 1:56:A:ALA:HB3 | 1:69:A:PHE:H | 10 | 0.26 |
| (1,170) | 1:56:A:ALA:HB1 | 1:69:A:PHE:H | 19 | 0.26 |
| (1,170) | 1:56:A:ALA:HB2 | 1:69:A:PHE:H | 19 | 0.26 |
| (1,170) | 1:56:A:ALA:HB3 | 1:69:A:PHE:H | 19 | 0.26 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 10 | 0.26 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 10 | 0.26 |
| (1,83) | 1:53:A:THR:HB | 1:76:A:MET:HB3 | 9 | 0.26 |
| (1,63) | 1:52:A:VAL:HG11 | 2:8:B:ILE:HA | 15 | 0.26 |
| (1,63) | 1:52:A:VAL:HG12 | 2:8:B:ILE:HA | 15 | 0.26 |
| (1,63) | 1:52:A:VAL:HG13 | 2:8:B:ILE:HA | 15 | 0.26 |
| (1,4046) | 2:19:B:GLN:HG2 | 2:21:B:MET:H | 17 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4046) | 2:19:B:GLN:HG3 | 2:21:B:MET:H | 17 | 0.25 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 7 | 0.25 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 7 | 0.25 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB2 | 2 | 0.25 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB3 | 2 | 0.25 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 20 | 0.25 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 20 | 0.25 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 18 | 0.25 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 18 | 0.25 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 8 | 0.25 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 8 | 0.25 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 8 | 0.25 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 8 | 0.25 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 8 | 0.25 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 8 | 0.25 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 18 | 0.25 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 18 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,3643) | 1:85:A:ASP:HB2 | 1:108:A:GLY:HA2 | 20 | 0.25 |
| (1,3643) | 1:85:A:ASP:HB3 | 1:108:A:GLY:HA2 | 20 | 0.25 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 15 | 0.25 |
| (1,3583) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 15 | 0.25 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD1 | 1 | 0.25 |
| (1,3532) | 1:63:A:TYR:HE1 | 2:10:B:TYR:HD2 | 1 | 0.25 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD1 | 1 | 0.25 |
| (1,3532) | 1:63:A:TYR:HE2 | 2:10:B:TYR:HD2 | 1 | 0.25 |
| (1,3526) | 1:69:A:PHE:HE1 | 2:21:B:MET:HB2 | 6 | 0.25 |
| (1,3526) | 1:69:A:PHE:HE2 | 2:21:B:MET:HB2 | 6 | 0.25 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 3 | 0.25 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 3 | 0.25 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 3 | 0.25 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 10 | 0.25 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 10 | 0.25 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 10 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD2 | 3 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD3 | 3 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD2 | 3 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD3 | 3 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD2 | 3 | 0.25 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD3 | 3 | 0.25 |
| (1,3387) | 2:8:B:ILE:HD11 | 2:21:B:MET:H | 12 | 0.25 |
| (1,3387) | 2:8:B:ILE:HD12 | 2:21:B:MET:H | 12 | 0.25 |
| (1,3387) | 2:8:B:ILE:HD13 | 2:21:B:MET:H | 12 | 0.25 |
| (1,3386) | 2:8:B:ILE:HD11 | 2:9:B:ILE:H | 6 | 0.25 |
| (1,3386) | 2:8:B:ILE:HD12 | 2:9:B:ILE:H | 6 | 0.25 |
| (1,3386) | 2:8:B:ILE:HD13 | 2:9:B:ILE:H | 6 | 0.25 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 4 | 0.25 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 4 | 0.25 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 4 | 0.25 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 8 | 0.25 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 12 | 0.25 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 18 | 0.25 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 14 | 0.25 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 14 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 9 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 9 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 9 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 9 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 9 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 9 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 11 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 11 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 11 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 11 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 11 | 0.25 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 11 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 2 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 2 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 2 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 2 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 2 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 2 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 17 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 17 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 17 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 17 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 17 | 0.25 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 17 | 0.25 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 4 | 0.25 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 4 | 0.25 |
| (1,3148) | 1:173:A:TYR:HD1 | 1:201:A:ILE:HA | 3 | 0.25 |
| (1,3148) | 1:173:A:TYR:HD2 | 1:201:A:ILE:HA | 3 | 0.25 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 12 | 0.25 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 12 | 0.25 |
| (1,3088) | 1:68:A:VAL:HA | 1:88:A:GLN:HE21 | 13 | 0.25 |
| (1,3067) | 1:167:A:ASP:HA | 1:196:A:ASN:HD21 | 4 | 0.25 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 7 | 0.25 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 3 | 0.25 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 19 | 0.25 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 15 | 0.25 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 15 | 0.25 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 15 | 0.25 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 10 | 0.25 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 10 | 0.25 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 10 | 0.25 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 1 | 0.25 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 1 | 0.25 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 14 | 0.25 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 20 | 0.25 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 8 | 0.25 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 13 | 0.25 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 14 | 0.25 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 16 | 0.25 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 15 | 0.25 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 15 | 0.25 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 15 | 0.25 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 11 | 0.25 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 3 | 0.25 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 4 | 0.25 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 4 | 0.25 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 4 | 0.25 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 4 | 0.25 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 4 | 0.25 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 4 | 0.25 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 16 | 0.25 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 16 | 0.25 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 16 | 0.25 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 8 | 0.25 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 2 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 2 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 2 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 2 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 4 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 4 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 4 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 7 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 7 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 7 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 13 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 13 | 0.25 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 11 | 0.25 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 13 | 0.25 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 13 | 0.25 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 13 | 0.25 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 10 | 0.25 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 17 | 0.25 |
| (1,2437) | 1:82:A:LEU:HG | 1:113:A:ASP:H | 6 | 0.25 |
| (1,2292) | 1:75:A:ILE:HG13 | 1:76:A:MET:H | 10 | 0.25 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 9 | 0.25 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 2 | 0.25 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 2 | 0.25 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 2 | 0.25 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 12 | 0.25 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 14 | 0.25 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 14 | 0.25 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 15 | 0.25 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 15 | 0.25 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 15 | 0.25 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 7 | 0.25 |
| (1,2074) | 1:223:A:THR:HB | 1:224:A:LEU:H | 9 | 0.25 |
| (1,2074) | 1:223:A:THR:HB | 1:224:A:LEU:H | 14 | 0.25 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 13 | 0.25 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 13 | 0.25 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 13 | 0.25 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 6 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 15 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 16 | 0.25 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 16 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 9 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 9 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 9 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 11 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 11 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 11 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 13 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 13 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 13 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 16 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 16 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 16 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 17 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 17 | 0.25 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 17 | 0.25 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 1 | 0.25 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 1 | 0.25 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 1 | 0.25 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 1 | 0.25 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 1 | 0.25 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 4 | 0.25 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 11 | 0.25 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 16 | 0.25 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 19 | 0.25 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 15 | 0.25 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 2 | 0.25 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 18 | 0.25 |
| (1,1713) | 1:194:A:ILE:HG21 | 1:195:A:ASN:HA | 9 | 0.25 |
| (1,1713) | 1:194:A:ILE:HG22 | 1:195:A:ASN:HA | 9 | 0.25 |
| (1,1713) | 1:194:A:ILE:HG23 | 1:195:A:ASN:HA | 9 | 0.25 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD11 | 9 | 0.25 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD12 | 9 | 0.25 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD13 | 9 | 0.25 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 14 | 0.25 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 14 | 0.25 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 14 | 0.25 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 17 | 0.25 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 17 | 0.25 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 17 | 0.25 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 15 | 0.25 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 18 | 0.25 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 7 | 0.25 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 7 | 0.25 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 7 | 0.25 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 12 | 0.25 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 12 | 0.25 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 12 | 0.25 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 18 | 0.25 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 18 | 0.25 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 18 | 0.25 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 7 | 0.25 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 7 | 0.25 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 7 | 0.25 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 9 | 0.25 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 6 | 0.25 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 18 | 0.25 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 4 | 0.25 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 4 | 0.25 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 4 | 0.25 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 8 | 0.25 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 8 | 0.25 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 8 | 0.25 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 15 | 0.25 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 15 | 0.25 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 15 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 2 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 2 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 2 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 3 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 3 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 3 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 14 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 14 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 14 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 19 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 19 | 0.25 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 19 | 0.25 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 16 | 0.25 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 16 | 0.25 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 16 | 0.25 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 16 | 0.25 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 16 | 0.25 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 16 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 4 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 4 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 4 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 7 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 7 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 7 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 9 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 9 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 9 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 20 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 20 | 0.25 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 20 | 0.25 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 6 | 0.25 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 2 | 0.25 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 3 | 0.25 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 4 | 0.25 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 11 | 0.25 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 15 | 0.25 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 9 | 0.25 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 9 | 0.25 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 19 | 0.25 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 19 | 0.25 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 7 | 0.25 |
| (1,1251) | 1:134:A:VAL:HA | 1:155:A:LYS:HE2 | 5 | 0.25 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 15 | 0.25 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 15 | 0.25 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 15 | 0.25 |
| (1,1220) | 1:53:A:THR:HG21 | 1:55:A:ASN:H | 8 | 0.25 |
| (1,1220) | 1:53:A:THR:HG22 | 1:55:A:ASN:H | 8 | 0.25 |
| (1,1220) | 1:53:A:THR:HG23 | 1:55:A:ASN:H | 8 | 0.25 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 3 | 0.25 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 19 | 0.25 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD2 | 7 | 0.25 |
| (1,1177) | 1:151:A:ALA:HB1 | 1:152:A:LYS:HD3 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD2 | 7 | 0.25 |
| (1,1177) | 1:151:A:ALA:HB2 | 1:152:A:LYS:HD3 | 7 | 0.25 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD2 | 7 | 0.25 |
| (1,1177) | 1:151:A:ALA:HB3 | 1:152:A:LYS:HD3 | 7 | 0.25 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 6 | 0.25 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 6 | 0.25 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 6 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 8 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 8 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 8 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 8 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 8 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 8 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 14 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 14 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 14 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 14 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 14 | 0.25 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 14 | 0.25 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 18 | 0.25 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 18 | 0.25 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 18 | 0.25 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 18 | 0.25 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 18 | 0.25 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 18 | 0.25 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 5 | 0.25 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 5 | 0.25 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 5 | 0.25 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 14 | 0.25 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 14 | 0.25 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 14 | 0.25 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 5 | 0.25 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 5 | 0.25 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 5 | 0.25 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 16 | 0.25 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 16 | 0.25 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 16 | 0.25 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 10 | 0.25 |
| (1,1057) | 1:139:A:SER:HB3 | 1:151:A:ALA:H | 19 | 0.25 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 2 | 0.25 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 2 | 0.25 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 18 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 18 | 0.25 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 18 | 0.25 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 6 | 0.25 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 6 | 0.25 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 6 | 0.25 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 13 | 0.25 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 13 | 0.25 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 13 | 0.25 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 17 | 0.25 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 10 | 0.25 |
| (1,675) | 1:103:A:THR:HG21 | 1:125:A:TRP:HZ2 | 8 | 0.25 |
| (1,675) | 1:103:A:THR:HG22 | 1:125:A:TRP:HZ2 | 8 | 0.25 |
| (1,675) | 1:103:A:THR:HG23 | 1:125:A:TRP:HZ2 | 8 | 0.25 |
| (1,675) | 1:103:A:THR:HG21 | 1:125:A:TRP:HZ2 | 18 | 0.25 |
| (1,675) | 1:103:A:THR:HG22 | 1:125:A:TRP:HZ2 | 18 | 0.25 |
| (1,675) | 1:103:A:THR:HG23 | 1:125:A:TRP:HZ2 | 18 | 0.25 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 9 | 0.25 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 9 | 0.25 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 12 | 0.25 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 12 | 0.25 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 2 | 0.25 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 2 | 0.25 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 2 | 0.25 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 18 | 0.25 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 18 | 0.25 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 18 | 0.25 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 18 | 0.25 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 18 | 0.25 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 18 | 0.25 |
| (1,564) | 1:74:A:ASP:HA | 1:75:A:ILE:HB | 14 | 0.25 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD23 | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD11 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD12 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD13 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD21 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD22 | 16 | 0.25 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD23 | 16 | 0.25 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 11 | 0.25 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 14 | 0.25 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 2 | 0.25 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 2 | 0.25 |
| (1,462) | 1:81:A:ARG:HA | 1:81:A:ARG:HD3 | 4 | 0.25 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 15 | 0.25 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 1 | 0.25 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 1 | 0.25 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 1 | 0.25 |
| (1,409) | 1:75:A:ILE:HG21 | 1:76:A:MET:HA | 15 | 0.25 |
| (1,409) | 1:75:A:ILE:HG22 | 1:76:A:MET:HA | 15 | 0.25 |
| (1,409) | 1:75:A:ILE:HG23 | 1:76:A:MET:HA | 15 | 0.25 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 14 | 0.25 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 14 | 0.25 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 14 | 0.25 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 12 | 0.25 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 20 | 0.25 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 20 | 0.25 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 20 | 0.25 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 19 | 0.25 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 19 | 0.25 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 19 | 0.25 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 19 | 0.25 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 19 | 0.25 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 19 | 0.25 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 1 | 0.25 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 1 | 0.25 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 1 | 0.25 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 4 | 0.25 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 4 | 0.25 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 4 | 0.25 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 14 | 0.25 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 15 | 0.25 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 15 | 0.25 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 15 | 0.25 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 11 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 11 | 0.25 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 11 | 0.25 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 3 | 0.25 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 3 | 0.25 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 3 | 0.25 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 14 | 0.25 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 14 | 0.25 |
| (1,142) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HB3 | 17 | 0.25 |
| (1,142) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HB3 | 17 | 0.25 |
| (1,142) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HB3 | 17 | 0.25 |
| (1,105) | 1:54:A:ILE:HB | 2:9:B:ILE:H | 4 | 0.25 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 20 | 0.25 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 20 | 0.25 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 7 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 7 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 7 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 7 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 7 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 7 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 15 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 15 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 15 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 15 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 15 | 0.24 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 15 | 0.24 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 13 | 0.24 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 13 | 0.24 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 13 | 0.24 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 13 | 0.24 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 13 | 0.24 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 13 | 0.24 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 3 | 0.24 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 3 | 0.24 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 3 | 0.24 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 3 | 0.24 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 3 | 0.24 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 2 | 0.24 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 2 | 0.24 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 15 | 0.24 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 15 | 0.24 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 15 | 0.24 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 15 | 0.24 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 15 | 0.24 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 15 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 3 | 0.24 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 3 | 0.24 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG21 | 9 | 0.24 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG22 | 9 | 0.24 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG23 | 9 | 0.24 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG21 | 9 | 0.24 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG22 | 9 | 0.24 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG23 | 9 | 0.24 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD1 | 11 | 0.24 |
| (1,3614) | 1:80:A:SER:HB2 | 1:112:A:TYR:HD2 | 11 | 0.24 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 11 | 0.24 |
| (1,3614) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 11 | 0.24 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 17 | 0.24 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 17 | 0.24 |
| (1,3493) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HA | 20 | 0.24 |
| (1,3493) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HA | 20 | 0.24 |
| (1,3493) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HA | 20 | 0.24 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 7 | 0.24 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 7 | 0.24 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 7 | 0.24 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 17 | 0.24 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 17 | 0.24 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 17 | 0.24 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 2 | 0.24 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 2 | 0.24 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 2 | 0.24 |
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 8 | 0.24 |
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 8 | 0.24 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 8 | 0.24 |
| (1,3415) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB3 | 11 | 0.24 |
| (1,3415) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB3 | 11 | 0.24 |
| (1,3415) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB3 | 11 | 0.24 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 18 | 0.24 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 18 | 0.24 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 18 | 0.24 |
| (1,3411) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB2 | 8 | 0.24 |
| (1,3411) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB2 | 8 | 0.24 |
| (1,3411) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB2 | 8 | 0.24 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 19 | 0.24 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 19 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 19 | 0.24 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 19 | 0.24 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 19 | 0.24 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 19 | 0.24 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 6 | 0.24 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 16 | 0.24 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 20 | 0.24 |
| (1,3327) | 2:10:B:TYR:HB2 | 2:21:B:MET:H | 18 | 0.24 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG2 | 20 | 0.24 |
| (1,3324) | 2:10:B:TYR:H | 2:20:B:ARG:HG3 | 20 | 0.24 |
| (1,3310) | 2:8:B:ILE:HD11 | 2:11:B:CYS:H | 16 | 0.24 |
| (1,3310) | 2:8:B:ILE:HD12 | 2:11:B:CYS:H | 16 | 0.24 |
| (1,3310) | 2:8:B:ILE:HD13 | 2:11:B:CYS:H | 16 | 0.24 |
| (1,3302) | 2:17:B:LYS:H | 2:17:B:LYS:HG3 | 16 | 0.24 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 3 | 0.24 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 7 | 0.24 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 10 | 0.24 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 4 | 0.24 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG11 | 9 | 0.24 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG12 | 9 | 0.24 |
| (1,3236) | 1:125:A:TRP:HZ3 | 1:134:A:VAL:HG13 | 9 | 0.24 |
| (1,3223) | 1:103:A:THR:HB | 1:125:A:TRP:HD1 | 8 | 0.24 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 16 | 0.24 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 16 | 0.24 |
| (1,3205) | 1:88:A:GLN:HG3 | 1:90:A:HIS:HE1 | 2 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 6 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 6 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 6 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 6 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 6 | 0.24 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 6 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 19 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 19 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 19 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 19 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 19 | 0.24 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 19 | 0.24 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 14 | 0.24 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 14 | 0.24 |
| (1,3134) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HD1 | 10 | 0.24 |
| (1,3134) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HD2 | 10 | 0.24 |
| (1,3134) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HD1 | 10 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3134) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HD2 | 10 | 0.24 |
| (1,3134) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HD1 | 10 | 0.24 |
| (1,3134) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HD2 | 10 | 0.24 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 6 | 0.24 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 17 | 0.24 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 11 | 0.24 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 5 | 0.24 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 14 | 0.24 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 8 | 0.24 |
| (1,3020) | 1:214:A:ALA:HB1 | 1:218:A:ALA:H | 12 | 0.24 |
| (1,3020) | 1:214:A:ALA:HB2 | 1:218:A:ALA:H | 12 | 0.24 |
| (1,3020) | 1:214:A:ALA:HB3 | 1:218:A:ALA:H | 12 | 0.24 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 14 | 0.24 |
| (1,3018) | 1:214:A:ALA:HA | 1:218:A:ALA:H | 16 | 0.24 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 1 | 0.24 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 1 | 0.24 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 1 | 0.24 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 10 | 0.24 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 13 | 0.24 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 19 | 0.24 |
| (1,2927) | 1:195:A:ASN:HB2 | 1:196:A:ASN:H | 19 | 0.24 |
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 1 | 0.24 |
| (1,2860) | 1:142:A:THR:HG21 | 1:183:A:ALA:H | 19 | 0.24 |
| (1,2860) | 1:142:A:THR:HG22 | 1:183:A:ALA:H | 19 | 0.24 |
| (1,2860) | 1:142:A:THR:HG23 | 1:183:A:ALA:H | 19 | 0.24 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 1 | 0.24 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 11 | 0.24 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 12 | 0.24 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 15 | 0.24 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 6 | 0.24 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 20 | 0.24 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 20 | 0.24 |
| (1,2761) | 1:167:A:ASP:H | 1:196:A:ASN:HB2 | 4 | 0.24 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 9 | 0.24 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 18 | 0.24 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 18 | 0.24 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 18 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 1 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 1 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 1 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 5 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 5 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 5 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 11 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 11 | 0.24 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 11 | 0.24 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 18 | 0.24 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 20 | 0.24 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 20 | 0.24 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 15 | 0.24 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 19 | 0.24 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 19 | 0.24 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 10 | 0.24 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 10 | 0.24 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 10 | 0.24 |
| (1,2372) | 1:92:A:LYS:H | 1:92:A:LYS:HG2 | 3 | 0.24 |
| (1,2372) | 1:92:A:LYS:H | 1:92:A:LYS:HG3 | 3 | 0.24 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 3 | 0.24 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 12 | 0.24 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 2 | 0.24 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 16 | 0.24 |
| (1,2087) | 1:198:A:THR:HB | 1:225:A:LYS:HB3 | 2 | 0.24 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 12 | 0.24 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 12 | 0.24 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 12 | 0.24 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 9 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 7 | 0.24 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 7 | 0.24 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 4 | 0.24 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 4 | 0.24 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 4 | 0.24 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 3 | 0.24 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 15 | 0.24 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 15 | 0.24 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 15 | 0.24 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 3 | 0.24 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 9 | 0.24 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 9 | 0.24 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 4 | 0.24 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 11 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 8 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 8 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 15 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 15 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 16 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 16 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 18 | 0.24 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 18 | 0.24 |
| (1,1795) | 1:201:A:ILE:HD11 | 1:202:A:THR:H | 10 | 0.24 |
| (1,1795) | 1:201:A:ILE:HD12 | 1:202:A:THR:H | 10 | 0.24 |
| (1,1795) | 1:201:A:ILE:HD13 | 1:202:A:THR:H | 10 | 0.24 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 2 | 0.24 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 6 | 0.24 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 7 | 0.24 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 8 | 0.24 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 4 | 0.24 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 1 | 0.24 |
| (1,1726) | 1:167:A:ASP:H | 1:196:A:ASN:HB3 | 18 | 0.24 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 15 | 0.24 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 8 | 0.24 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 8 | 0.24 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 8 | 0.24 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 12 | 0.24 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 10 | 0.24 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 10 | 0.24 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 10 | 0.24 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 10 | 0.24 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 10 | 0.24 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 10 | 0.24 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 6 | 0.24 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 10 | 0.24 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 20 | 0.24 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 8 | 0.24 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 3 | 0.24 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 5 | 0.24 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 5 | 0.24 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 5 | 0.24 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 20 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 2 | 0.24 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 2 | 0.24 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 2 | 0.24 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 1 | 0.24 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 1 | 0.24 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 1 | 0.24 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 1 | 0.24 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 1 | 0.24 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 1 | 0.24 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 16 | 0.24 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 16 | 0.24 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 16 | 0.24 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 5 | 0.24 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 14 | 0.24 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 19 | 0.24 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 19 | 0.24 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 19 | 0.24 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 11 | 0.24 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 3 | 0.24 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 17 | 0.24 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 2 | 0.24 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 2 | 0.24 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 2 | 0.24 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 6 | 0.24 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 12 | 0.24 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 13 | 0.24 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 1 | 0.24 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 4 | 0.24 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 4 | 0.24 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 10 | 0.24 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 20 | 0.24 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 9 | 0.24 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 20 | 0.24 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 10 | 0.24 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 10 | 0.24 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 10 | 0.24 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 2 | 0.24 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 8 | 0.24 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 15 | 0.24 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 15 | 0.24 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 15 | 0.24 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 18 | 0.24 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 7 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 1 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 1 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 1 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 1 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 1 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 1 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 13 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 13 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 13 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 13 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 13 | 0.24 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 13 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 1 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 1 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 1 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 9 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 9 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 9 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 15 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 15 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 15 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 18 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 18 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 18 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 19 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 19 | 0.24 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 19 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 7 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 7 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 7 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 7 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 7 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 7 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 18 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 18 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 18 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 18 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 18 | 0.24 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 18 | 0.24 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 18 | 0.24 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 18 | 0.24 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 8 | 0.24 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 6 | 0.24 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 6 | 0.24 |
| (1,1006) | 1:136:A:TYR:HB3 | 1:152:A:LYS:HA | 5 | 0.24 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 9 | 0.24 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 9 | 0.24 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 9 | 0.24 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 1 | 0.24 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 3 | 0.24 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 19 | 0.24 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 2 | 0.24 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 2 | 0.24 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 2 | 0.24 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 3 | 0.24 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 3 | 0.24 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 3 | 0.24 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 12 | 0.24 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 12 | 0.24 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 12 | 0.24 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 7 | 0.24 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 7 | 0.24 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 7 | 0.24 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 17 | 0.24 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 17 | 0.24 |
| (1,780) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG12 | 14 | 0.24 |
| (1,776) | 1:113:A:ASP:HA | 1:118:A:ILE:HG12 | 9 | 0.24 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 11 | 0.24 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 7 | 0.24 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 12 | 0.24 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 19 | 0.24 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG21 | 20 | 0.24 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG22 | 20 | 0.24 |
| (1,658) | 1:103:A:THR:HA | 1:104:A:VAL:HG23 | 20 | 0.24 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 2 | 0.24 |
| (1,526) | 1:87:A:VAL:HG11 | 1:104:A:VAL:HA | 5 | 0.24 |
| (1,526) | 1:87:A:VAL:HG12 | 1:104:A:VAL:HA | 5 | 0.24 |
| (1,526) | 1:87:A:VAL:HG13 | 1:104:A:VAL:HA | 5 | 0.24 |
| (1,526) | 1:87:A:VAL:HG21 | 1:104:A:VAL:HA | 5 | 0.24 |
| (1,526) | 1:87:A:VAL:HG22 | 1:104:A:VAL:HA | 5 | 0.24 |
| (1,526) | 1:87:A:VAL:HG23 | 1:104:A:VAL:HA | 5 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 9 | 0.24 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 6 | 0.24 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 12 | 0.24 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 12 | 0.24 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 12 | 0.24 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 12 | 0.24 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 12 | 0.24 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 12 | 0.24 |
| (1,330) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HA | 18 | 0.24 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 12 | 0.24 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 14 | 0.24 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 14 | 0.24 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 14 | 0.24 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 12 | 0.24 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 12 | 0.24 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 12 | 0.24 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 12 | 0.24 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 2 | 0.24 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 4 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 4 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 4 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 4 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 16 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 16 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 16 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 19 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 19 | 0.24 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 19 | 0.24 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 3 | 0.24 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 3 | 0.24 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 3 | 0.24 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 11 | 0.24 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 11 | 0.24 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 11 | 0.24 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 2 | 0.24 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 2 | 0.24 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 5 | 0.24 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 5 | 0.24 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 6 | 0.24 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 6 | 0.24 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 10 | 0.24 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 10 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 20 | 0.24 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 20 | 0.24 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 13 | 0.24 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 13 | 0.24 |
| (1,79) | 1:70:A:THR:HA | 1:86:A:GLU:HB3 | 2 | 0.24 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 2 | 0.23 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 2 | 0.23 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 10 | 0.23 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 10 | 0.23 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 10 | 0.23 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 10 | 0.23 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 10 | 0.23 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 10 | 0.23 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 9 | 0.23 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 9 | 0.23 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 9 | 0.23 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 9 | 0.23 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 9 | 0.23 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 9 | 0.23 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 11 | 0.23 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 11 | 0.23 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 2 | 0.23 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 2 | 0.23 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 13 | 0.23 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 13 | 0.23 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 13 | 0.23 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 13 | 0.23 |
| (1,3605) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HA | 13 | 0.23 |
| (1,3605) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HA | 13 | 0.23 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB1 | 1 | 0.23 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB2 | 1 | 0.23 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB3 | 1 | 0.23 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB1 | 1 | 0.23 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB2 | 1 | 0.23 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB3 | 1 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3505) | 1:51:A:PRO:HB3 | 2:7:B:PRO:HD3 | 4 | 0.23 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 17 | 0.23 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 17 | 0.23 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 17 | 0.23 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 17 | 0.23 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 17 | 0.23 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 17 | 0.23 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 3 | 0.23 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 3 | 0.23 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 3 | 0.23 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 3 | 0.23 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 3 | 0.23 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 3 | 0.23 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 13 | 0.23 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 13 | 0.23 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 13 | 0.23 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 13 | 0.23 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 13 | 0.23 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 13 | 0.23 |
| (1,3346) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB2 | 15 | 0.23 |
| (1,3346) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB2 | 15 | 0.23 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 4 | 0.23 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 11 | 0.23 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 1 | 0.23 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 17 | 0.23 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 17 | 0.23 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 14 | 0.23 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB1 | 17 | 0.23 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB2 | 17 | 0.23 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB3 | 17 | 0.23 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 17 | 0.23 |
| (1,3208) | 1:126:A:ALA:HB1 | 1:133:A:TRP:HD1 | 15 | 0.23 |
| (1,3208) | 1:126:A:ALA:HB2 | 1:133:A:TRP:HD1 | 15 | 0.23 |
| (1,3208) | 1:126:A:ALA:HB3 | 1:133:A:TRP:HD1 | 15 | 0.23 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 12 | 0.23 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 12 | 0.23 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 12 | 0.23 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 12 | 0.23 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 12 | 0.23 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 12 | 0.23 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 13 | 0.23 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 13 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 13 | 0.23 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 13 | 0.23 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 13 | 0.23 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 13 | 0.23 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 4 | 0.23 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 4 | 0.23 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 4 | 0.23 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 4 | 0.23 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 4 | 0.23 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 4 | 0.23 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 17 | 0.23 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 17 | 0.23 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 17 | 0.23 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 7 | 0.23 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 16 | 0.23 |
| (1,3079) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 18 | 0.23 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 3 | 0.23 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 18 | 0.23 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 9 | 0.23 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 13 | 0.23 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 13 | 0.23 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 13 | 0.23 |
| (1,2968) | 1:202:A:THR:H | 1:205:A:LYS:HG2 | 17 | 0.23 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 20 | 0.23 |
| (1,2950) | 1:198:A:THR:HA | 1:199:A:GLY:H | 17 | 0.23 |
| (1,2932) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 5 | 0.23 |
| (1,2932) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 5 | 0.23 |
| (1,2932) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 5 | 0.23 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 1 | 0.23 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 2 | 0.23 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 14 | 0.23 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 6 | 0.23 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 9 | 0.23 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 19 | 0.23 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 20 | 0.23 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 11 | 0.23 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 1 | 0.23 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 16 | 0.23 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 17 | 0.23 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 14 | 0.23 |
| (1,2761) | 1:167:A:ASP:H | 1:196:A:ASN:HB2 | 10 | 0.23 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 5 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 5 | 0.23 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 5 | 0.23 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 19 | 0.23 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 19 | 0.23 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 19 | 0.23 |
| (1,2752) | 1:154:A:ILE:HA | 1:166:A:ASP:H | 12 | 0.23 |
| (1,2725) | 1:159:A:ASN:H | 1:162:A:THR:HB | 15 | 0.23 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 15 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 12 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 12 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 12 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 12 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 12 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 12 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 16 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 16 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 16 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 16 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 16 | 0.23 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 16 | 0.23 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 10 | 0.23 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 20 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 5 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 5 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 5 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 8 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 8 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 8 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 14 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 14 | 0.23 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 14 | 0.23 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 1 | 0.23 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 1 | 0.23 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 1 | 0.23 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 3 | 0.23 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 6 | 0.23 |
| (1,2605) | 1:142:A:THR:H | 1:148:A:SER:HA | 19 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 5 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 5 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 10 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 10 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 14 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 14 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 17 | 0.23 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 17 | 0.23 |
| (1,2506) | 1:147:A:GLY:HA2 | 1:179:A:LEU:H | 15 | 0.23 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 11 | 0.23 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 16 | 0.23 |
| (1,2478) | 1:112:A:TYR:HB2 | 1:119:A:LEU:H | 19 | 0.23 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 3 | 0.23 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 3 | 0.23 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 1 | 0.23 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 19 | 0.23 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 19 | 0.23 |
| (1,2288) | 1:75:A:ILE:HB | 1:76:A:MET:H | 7 | 0.23 |
| (1,2279) | 1:75:A:ILE:H | 1:84:A:ALA:H | 3 | 0.23 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 16 | 0.23 |
| (1,2217) | 1:62:A:ASP:H | 1:66:A:ASP:HB2 | 3 | 0.23 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 20 | 0.23 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 17 | 0.23 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 11 | 0.23 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 11 | 0.23 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 11 | 0.23 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 5 | 0.23 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 5 | 0.23 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 1 | 0.23 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 1 | 0.23 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 1 | 0.23 |
| (1,2009) | 1:216:A:LEU:HD11 | 1:217:A:GLY:H | 3 | 0.23 |
| (1,2009) | 1:216:A:LEU:HD12 | 1:217:A:GLY:H | 3 | 0.23 |
| (1,2009) | 1:216:A:LEU:HD13 | 1:217:A:GLY:H | 3 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 19 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 19 | 0.23 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 19 | 0.23 |
| (1,1922) | 1:209:A:LEU:HD21 | 1:210:A:LYS:H | 1 | 0.23 |
| (1,1922) | 1:209:A:LEU:HD22 | 1:210:A:LYS:H | 1 | 0.23 |
| (1,1922) | 1:209:A:LEU:HD23 | 1:210:A:LYS:H | 1 | 0.23 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 18 | 0.23 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD2 | 17 | 0.23 |
| (1,1887) | 1:207:A:THR:HB | 1:208:A:LYS:HD3 | 17 | 0.23 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 2 | 0.23 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 6 | 0.23 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 14 | 0.23 |
| (1,1802) | 1:201:A:ILE:HD11 | 1:205:A:LYS:HG3 | 1 | 0.23 |
| (1,1802) | 1:201:A:ILE:HD12 | 1:205:A:LYS:HG3 | 1 | 0.23 |
| (1,1802) | 1:201:A:ILE:HD13 | 1:205:A:LYS:HG3 | 1 | 0.23 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 1 | 0.23 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 8 | 0.23 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 9 | 0.23 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 17 | 0.23 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 18 | 0.23 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 11 | 0.23 |
| (1,1722) | 1:195:A:ASN:HB3 | 1:196:A:ASN:HA | 19 | 0.23 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 11 | 0.23 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 12 | 0.23 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 12 | 0.23 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 12 | 0.23 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 19 | 0.23 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 19 | 0.23 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 19 | 0.23 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 16 | 0.23 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 9 | 0.23 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 9 | 0.23 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 9 | 0.23 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 11 | 0.23 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 11 | 0.23 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 11 | 0.23 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 13 | 0.23 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 13 | 0.23 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 2 | 0.23 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 7 | 0.23 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 17 | 0.23 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 10 | 0.23 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 10 | 0.23 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 11 | 0.23 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 11 | 0.23 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 11 | 0.23 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 11 | 0.23 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 11 | 0.23 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 11 | 0.23 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 18 | 0.23 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 11 | 0.23 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 11 | 0.23 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 11 | 0.23 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 18 | 0.23 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 18 | 0.23 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 18 | 0.23 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 2 | 0.23 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 5 | 0.23 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 15 | 0.23 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 16 | 0.23 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 17 | 0.23 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 1 | 0.23 |
| (1,1363) | 1:153:A:VAL:H | 1:166:A:ASP:HB2 | 9 | 0.23 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 4 | 0.23 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 15 | 0.23 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 15 | 0.23 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 18 | 0.23 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 18 | 0.23 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 8 | 0.23 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 8 | 0.23 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 8 | 0.23 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 8 | 0.23 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 2 | 0.23 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 2 | 0.23 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 2 | 0.23 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 9 | 0.23 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 6 | 0.23 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 12 | 0.23 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 12 | 0.23 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 12 | 0.23 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD2 | 6 | 0.23 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD3 | 6 | 0.23 |
| (1,1191) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HA | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 2 | 0.23 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 2 | 0.23 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 2 | 0.23 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 17 | 0.23 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 17 | 0.23 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 17 | 0.23 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 11 | 0.23 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 11 | 0.23 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 11 | 0.23 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 1 | 0.23 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 6 | 0.23 |
| (1,1100) | 1:141:A:GLU:HB3 | 1:148:A:SER:HA | 9 | 0.23 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 6 | 0.23 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 6 | 0.23 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 6 | 0.23 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 6 | 0.23 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 6 | 0.23 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 6 | 0.23 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 11 | 0.23 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 11 | 0.23 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 11 | 0.23 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 11 | 0.23 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 11 | 0.23 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 11 | 0.23 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 11 | 0.23 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 11 | 0.23 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 11 | 0.23 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 7 | 0.23 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 7 | 0.23 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 7 | 0.23 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 11 | 0.23 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 14 | 0.23 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 17 | 0.23 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 7 | 0.23 |
| (1,991) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG13 | 3 | 0.23 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 15 | 0.23 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 2 | 0.23 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 8 | 0.23 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 14 | 0.23 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 20 | 0.23 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 18 | 0.23 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 8 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 8 | 0.23 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 8 | 0.23 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 8 | 0.23 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 8 | 0.23 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 8 | 0.23 |
| (1,828) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HE1 | 20 | 0.23 |
| (1,828) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HE1 | 20 | 0.23 |
| (1,828) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HE1 | 20 | 0.23 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 13 | 0.23 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 13 | 0.23 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 13 | 0.23 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 11 | 0.23 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 11 | 0.23 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 11 | 0.23 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 11 | 0.23 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 6 | 0.23 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 11 | 0.23 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 12 | 0.23 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 19 | 0.23 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 5 | 0.23 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 6 | 0.23 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 15 | 0.23 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 3 | 0.23 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 3 | 0.23 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 3 | 0.23 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 3 | 0.23 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 3 | 0.23 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 3 | 0.23 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 12 | 0.23 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 12 | 0.23 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 12 | 0.23 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 13 | 0.23 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 13 | 0.23 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 13 | 0.23 |
| (1,541) | 1:94:A:ALA:H | 1:97:A:GLN:HG3 | 4 | 0.23 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 2 | 0.23 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 8 | 0.23 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 17 | 0.23 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 18 | 0.23 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 12 | 0.23 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 1 | 0.23 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 9 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,513) | 1:123:A:LYS:HB3 | 1:123:A:LYS:HD3 | 11 | 0.23 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 11 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 3 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 3 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 3 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 8 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 8 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 8 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD11 | 14 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD12 | 14 | 0.23 |
| (1,390) | 1:135:A:PHE:H | 1:154:A:ILE:HD13 | 14 | 0.23 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 9 | 0.23 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 9 | 0.23 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 9 | 0.23 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 9 | 0.23 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 9 | 0.23 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 9 | 0.23 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 9 | 0.23 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 9 | 0.23 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 9 | 0.23 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 1 | 0.23 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 1 | 0.23 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 1 | 0.23 |
| (1,322) | 1:71:A:GLY:HA2 | 1:72:A:SER:HA | 15 | 0.23 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 15 | 0.23 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 15 | 0.23 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 15 | 0.23 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 15 | 0.23 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 15 | 0.23 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 15 | 0.23 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 16 | 0.23 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 16 | 0.23 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 16 | 0.23 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 19 | 0.23 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 19 | 0.23 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 19 | 0.23 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 7 | 0.23 |
| (1,255) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 7 | 0.23 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 13 | 0.23 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 13 | 0.23 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 13 | 0.23 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 7 | 0.23 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 7 | 0.23 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE1 | 7 | 0.23 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE2 | 7 | 0.23 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 18 | 0.23 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 18 | 0.23 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 18 | 0.23 |
| (1,101) | 1:53:A:THR:HG21 | 1:55:A:ASN:HD21 | 11 | 0.23 |
| (1,101) | 1:53:A:THR:HG22 | 1:55:A:ASN:HD21 | 11 | 0.23 |
| (1,101) | 1:53:A:THR:HG23 | 1:55:A:ASN:HD21 | 11 | 0.23 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 9 | 0.23 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 9 | 0.23 |
| (1,80) | 1:53:A:THR:HA | 2:9:B:ILE:HA | 18 | 0.23 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 7 | 0.23 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 7 | 0.23 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 5 | 0.23 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 16 | 0.23 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD2 | 12 | 0.22 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD3 | 12 | 0.22 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 12 | 0.22 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 12 | 0.22 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB2 | 5 | 0.22 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB3 | 5 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 5 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 5 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 5 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 5 | 0.22 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 5 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 5 | 0.22 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 6 | 0.22 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 6 | 0.22 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 6 | 0.22 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 6 | 0.22 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 6 | 0.22 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 6 | 0.22 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 12 | 0.22 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 12 | 0.22 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 12 | 0.22 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 12 | 0.22 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 12 | 0.22 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 12 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 6 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 6 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 6 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 6 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 6 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 6 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 12 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 12 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 12 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 12 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 12 | 0.22 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 12 | 0.22 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 13 | 0.22 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 13 | 0.22 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 13 | 0.22 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 13 | 0.22 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 13 | 0.22 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 13 | 0.22 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 14 | 0.22 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 14 | 0.22 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 14 | 0.22 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 14 | 0.22 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 14 | 0.22 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 14 | 0.22 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG21 | 19 | 0.22 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG22 | 19 | 0.22 |
| (1,3709) | 1:102:A:ARG:HG2 | 2:8:B:ILE:HG23 | 19 | 0.22 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG21 | 19 | 0.22 |
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG22 | 19 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3709) | 1:102:A:ARG:HG3 | 2:8:B:ILE:HG23 | 19 | 0.22 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 15 | 0.22 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 15 | 0.22 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 15 | 0.22 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 15 | 0.22 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 15 | 0.22 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 15 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HG2 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD11 | 1:91:A:GLN:HG3 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HG2 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD12 | 1:91:A:GLN:HG3 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HG2 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD13 | 1:91:A:GLN:HG3 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HG2 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD21 | 1:91:A:GLN:HG3 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HG2 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD22 | 1:91:A:GLN:HG3 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HG2 | 8 | 0.22 |
| (1,3663) | 1:89:A:LEU:HD23 | 1:91:A:GLN:HG3 | 8 | 0.22 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 17 | 0.22 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 17 | 0.22 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 1 | 0.22 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 1 | 0.22 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 1 | 0.22 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 1 | 0.22 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 1 | 0.22 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 1 | 0.22 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 3 | 0.22 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 3 | 0.22 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 3 | 0.22 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD11 | 4 | 0.22 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD12 | 4 | 0.22 |
| (1,3413) | 2:8:B:ILE:HG13 | 2:9:B:ILE:HD13 | 4 | 0.22 |
| (1,3396) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HA | 6 | 0.22 |
| (1,3396) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HA | 6 | 0.22 |
| (1,3396) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HA | 6 | 0.22 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 4 | 0.22 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 4 | 0.22 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 14 | 0.22 |
| (1,3248) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HE1 | 3 | 0.22 |
| (1,3248) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HE1 | 3 | 0.22 |
| (1,3248) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HE1 | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3216) | 1:133:A:TRP:HZ2 | 1:163:A:LEU:HD11 | 12 | 0.22 |
| (1,3216) | 1:133:A:TRP:HZ2 | 1:163:A:LEU:HD12 | 12 | 0.22 |
| (1,3216) | 1:133:A:TRP:HZ2 | 1:163:A:LEU:HD13 | 12 | 0.22 |
| (1,3216) | 1:133:A:TRP:HZ2 | 1:163:A:LEU:HD21 | 12 | 0.22 |
| (1,3216) | 1:133:A:TRP:HZ2 | 1:163:A:LEU:HD22 | 12 | 0.22 |
| (1,3216) | 1:133:A:TRP:HZ2 | 1:163:A:LEU:HD23 | 12 | 0.22 |
| (1,3191) | 1:170:A:PHE:HE1 | 1:179:A:LEU:HB2 | 19 | 0.22 |
| (1,3191) | 1:170:A:PHE:HE2 | 1:179:A:LEU:HB2 | 19 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 7 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 7 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 7 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 7 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 7 | 0.22 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 7 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 20 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 20 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 20 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 20 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 20 | 0.22 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 20 | 0.22 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG11 | 20 | 0.22 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG12 | 20 | 0.22 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG13 | 20 | 0.22 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG11 | 20 | 0.22 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG12 | 20 | 0.22 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG13 | 20 | 0.22 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 13 | 0.22 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 13 | 0.22 |
| (1,3096) | 1:60:A:LYS:HE3 | 1:61:A:GLY:H | 14 | 0.22 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 4 | 0.22 |
| (1,3091) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 14 | 0.22 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 19 | 0.22 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 5 | 0.22 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 18 | 0.22 |
| (1,3027) | 1:190:A:LYS:HB3 | 1:219:A:THR:H | 20 | 0.22 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 2 | 0.22 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 2 | 0.22 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 2 | 0.22 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 13 | 0.22 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 9 | 0.22 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 9 | 0.22 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 7 | 0.22 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 12 | 0.22 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 15 | 0.22 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 16 | 0.22 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 18 | 0.22 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 5 | 0.22 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 18 | 0.22 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 1 | 0.22 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 1 | 0.22 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 1 | 0.22 |
| (1,2840) | 1:176:A:ALA:HB1 | 1:178:A:ALA:H | 7 | 0.22 |
| (1,2840) | 1:176:A:ALA:HB2 | 1:178:A:ALA:H | 7 | 0.22 |
| (1,2840) | 1:176:A:ALA:HB3 | 1:178:A:ALA:H | 7 | 0.22 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 2 | 0.22 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 13 | 0.22 |
| (1,2788) | 1:172:A:SER:H | 1:175:A:ASN:H | 14 | 0.22 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 6 | 0.22 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 6 | 0.22 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 6 | 0.22 |
| (1,2752) | 1:154:A:ILE:HA | 1:166:A:ASP:H | 17 | 0.22 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 18 | 0.22 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 19 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 4 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 4 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 4 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 4 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 4 | 0.22 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 4 | 0.22 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 3 | 0.22 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 3 | 0.22 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 3 | 0.22 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 13 | 0.22 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 13 | 0.22 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 13 | 0.22 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 17 | 0.22 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 19 | 0.22 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 19 | 0.22 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 19 | 0.22 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 18 | 0.22 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 15 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 6 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 6 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 7 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 7 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 8 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 8 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 16 | 0.22 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 16 | 0.22 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 18 | 0.22 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 18 | 0.22 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 18 | 0.22 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 5 | 0.22 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 13 | 0.22 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 15 | 0.22 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 16 | 0.22 |
| (1,2510) | 1:202:A:THR:HG21 | 1:205:A:LYS:H | 12 | 0.22 |
| (1,2510) | 1:202:A:THR:HG22 | 1:205:A:LYS:H | 12 | 0.22 |
| (1,2510) | 1:202:A:THR:HG23 | 1:205:A:LYS:H | 12 | 0.22 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 4 | 0.22 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 4 | 0.22 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 4 | 0.22 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 11 | 0.22 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 11 | 0.22 |
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 1 | 0.22 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 1 | 0.22 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 1 | 0.22 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 4 | 0.22 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 5 | 0.22 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 13 | 0.22 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 19 | 0.22 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 18 | 0.22 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 18 | 0.22 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 18 | 0.22 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 20 | 0.22 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 14 | 0.22 |
| (1,2216) | 1:62:A:ASP:H | 1:66:A:ASP:HB3 | 12 | 0.22 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 18 | 0.22 |
| (1,2120) | 1:74:A:ASP:HA | 1:83:A:GLN:HG3 | 14 | 0.22 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 11 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 11 | 0.22 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 11 | 0.22 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 8 | 0.22 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 8 | 0.22 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 8 | 0.22 |
| (1,2074) | 1:223:A:THR:HB | 1:224:A:LEU:H | 3 | 0.22 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 10 | 0.22 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 10 | 0.22 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 10 | 0.22 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 10 | 0.22 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 10 | 0.22 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 10 | 0.22 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD2 | 10 | 0.22 |
| (1,2043) | 1:198:A:THR:HG21 | 1:225:A:LYS:HD3 | 10 | 0.22 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD2 | 10 | 0.22 |
| (1,2043) | 1:198:A:THR:HG22 | 1:225:A:LYS:HD3 | 10 | 0.22 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD2 | 10 | 0.22 |
| (1,2043) | 1:198:A:THR:HG23 | 1:225:A:LYS:HD3 | 10 | 0.22 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 8 | 0.22 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 16 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 5 | 0.22 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 5 | 0.22 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 7 | 0.22 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 19 | 0.22 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 20 | 0.22 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE2 | 12 | 0.22 |
| (1,1864) | 1:205:A:LYS:H | 1:205:A:LYS:HE3 | 12 | 0.22 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 3 | 0.22 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 3 | 0.22 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 3 | 0.22 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 11 | 0.22 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 2 | 0.22 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 2 | 0.22 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 9 | 0.22 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 2 | 0.22 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 16 | 0.22 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 3 | 0.22 |
| (1,1713) | 1:194:A:ILE:HG21 | 1:195:A:ASN:HA | 12 | 0.22 |
| (1,1713) | 1:194:A:ILE:HG22 | 1:195:A:ASN:HA | 12 | 0.22 |
| (1,1713) | 1:194:A:ILE:HG23 | 1:195:A:ASN:HA | 12 | 0.22 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 10 | 0.22 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 10 | 0.22 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 10 | 0.22 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 16 | 0.22 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 16 | 0.22 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 16 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 2 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 2 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 2 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 12 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 12 | 0.22 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 12 | 0.22 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 10 | 0.22 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 8 | 0.22 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 8 | 0.22 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 8 | 0.22 |
| (1,1607) | 1:168:A:ALA:HB1 | 1:169:A:THR:HA | 3 | 0.22 |
| (1,1607) | 1:168:A:ALA:HB2 | 1:169:A:THR:HA | 3 | 0.22 |
| (1,1607) | 1:168:A:ALA:HB3 | 1:169:A:THR:HA | 3 | 0.22 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 6 | 0.22 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 6 | 0.22 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 6 | 0.22 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 10 | 0.22 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 10 | 0.22 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 10 | 0.22 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 16 | 0.22 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 16 | 0.22 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 16 | 0.22 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 9 | 0.22 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 17 | 0.22 |
| (1,1568) | 1:184:A:ILE:HG21 | 1:216:A:LEU:H | 9 | 0.22 |
| (1,1568) | 1:184:A:ILE:HG22 | 1:216:A:LEU:H | 9 | 0.22 |
| (1,1568) | 1:184:A:ILE:HG23 | 1:216:A:LEU:H | 9 | 0.22 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 11 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 6 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 6 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 6 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 15 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 15 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 15 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 18 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 18 | 0.22 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 18 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 11 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 11 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 11 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 14 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 14 | 0.22 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 14 | 0.22 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 12 | 0.22 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 15 | 0.22 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 6 | 0.22 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 6 | 0.22 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 6 | 0.22 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 6 | 0.22 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 6 | 0.22 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 6 | 0.22 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 10 | 0.22 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 10 | 0.22 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 10 | 0.22 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 10 | 0.22 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 10 | 0.22 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 10 | 0.22 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 20 | 0.22 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 8 | 0.22 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 12 | 0.22 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 15 | 0.22 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 19 | 0.22 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 4 | 0.22 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 9 | 0.22 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 11 | 0.22 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 16 | 0.22 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 11 | 0.22 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 19 | 0.22 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 12 | 0.22 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 12 | 0.22 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 12 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 8 | 0.22 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 9 | 0.22 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 3 | 0.22 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 3 | 0.22 |
| (1,1321) | 1:158:A:ASP:HB2 | 1:162:A:THR:HA | 12 | 0.22 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD2 | 16 | 0.22 |
| (1,1298) | 1:160:A:GLY:HA3 | 1:161:A:LYS:HD3 | 16 | 0.22 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 4 | 0.22 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 4 | 0.22 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 4 | 0.22 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 4 | 0.22 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 6 | 0.22 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 6 | 0.22 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 6 | 0.22 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 14 | 0.22 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 17 | 0.22 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 4 | 0.22 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 4 | 0.22 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 4 | 0.22 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 4 | 0.22 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 10 | 0.22 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 10 | 0.22 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 10 | 0.22 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 9 | 0.22 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 15 | 0.22 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 20 | 0.22 |
| (1,967) | 1:134:A:VAL:HA | 1:155:A:LYS:HB3 | 17 | 0.22 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 6 | 0.22 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 6 | 0.22 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 14 | 0.22 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 14 | 0.22 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 20 | 0.22 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 20 | 0.22 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 13 | 0.22 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 10 | 0.22 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 10 | 0.22 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 10 | 0.22 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 12 | 0.22 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 10 | 0.22 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 17 | 0.22 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 17 | 0.22 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 17 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 17 | 0.22 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 17 | 0.22 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 17 | 0.22 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 8 | 0.22 |
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 4 | 0.22 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 9 | 0.22 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 9 | 0.22 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 3 | 0.22 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 3 | 0.22 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 14 | 0.22 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 14 | 0.22 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 14 | 0.22 |
| (1,538) | 1:68:A:VAL:HG11 | 1:88:A:GLN:HG3 | 5 | 0.22 |
| (1,538) | 1:68:A:VAL:HG12 | 1:88:A:GLN:HG3 | 5 | 0.22 |
| (1,538) | 1:68:A:VAL:HG13 | 1:88:A:GLN:HG3 | 5 | 0.22 |
| (1,538) | 1:68:A:VAL:HG21 | 1:88:A:GLN:HG3 | 5 | 0.22 |
| (1,538) | 1:68:A:VAL:HG22 | 1:88:A:GLN:HG3 | 5 | 0.22 |
| (1,538) | 1:68:A:VAL:HG23 | 1:88:A:GLN:HG3 | 5 | 0.22 |
| (1,538) | 1:68:A:VAL:HG11 | 1:88:A:GLN:HG3 | 6 | 0.22 |
| (1,538) | 1:68:A:VAL:HG12 | 1:88:A:GLN:HG3 | 6 | 0.22 |
| (1,538) | 1:68:A:VAL:HG13 | 1:88:A:GLN:HG3 | 6 | 0.22 |
| (1,538) | 1:68:A:VAL:HG21 | 1:88:A:GLN:HG3 | 6 | 0.22 |
| (1,538) | 1:68:A:VAL:HG22 | 1:88:A:GLN:HG3 | 6 | 0.22 |
| (1,538) | 1:68:A:VAL:HG23 | 1:88:A:GLN:HG3 | 6 | 0.22 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 1 | 0.22 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 4 | 0.22 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 13 | 0.22 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 16 | 0.22 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 15 | 0.22 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 15 | 0.22 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 16 | 0.22 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 1 | 0.22 |
| (1,418) | 1:53:A:THR:H | 1:76:A:MET:HB3 | 10 | 0.22 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 2 | 0.22 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 2 | 0.22 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 2 | 0.22 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD11 | 5 | 0.22 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD12 | 5 | 0.22 |
| (1,396) | 1:153:A:VAL:H | 1:154:A:ILE:HD13 | 5 | 0.22 |
| (1,317) | 1:218:A:ALA:HB1 | 1:220:A:LEU:HA | 3 | 0.22 |
| (1,317) | 1:218:A:ALA:HB2 | 1:220:A:LEU:HA | 3 | 0.22 |
| (1,317) | 1:218:A:ALA:HB3 | 1:220:A:LEU:HA | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 15 | 0.22 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 15 | 0.22 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 15 | 0.22 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 13 | 0.22 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 13 | 0.22 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 13 | 0.22 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 17 | 0.22 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 17 | 0.22 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 17 | 0.22 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 20 | 0.22 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 20 | 0.22 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 20 | 0.22 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 15 | 0.22 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 19 | 0.22 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 1 | 0.22 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 1 | 0.22 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 1 | 0.22 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 11 | 0.22 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 11 | 0.22 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 11 | 0.22 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 17 | 0.22 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 17 | 0.22 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 17 | 0.22 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 1 | 0.22 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 1 | 0.22 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 1 | 0.22 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 15 | 0.22 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 15 | 0.22 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 15 | 0.22 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 19 | 0.22 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 19 | 0.22 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 19 | 0.22 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 3 | 0.22 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 3 | 0.22 |
| (1,61) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG13 | 18 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,61) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG13 | 18 | 0.22 |
| (1,61) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG13 | 18 | 0.22 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 1 | 0.22 |
| (1,33) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB3 | 6 | 0.22 |
| (1,33) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB3 | 6 | 0.22 |
| (1,33) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB3 | 6 | 0.22 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD2 | 10 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD3 | 10 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 10 | 0.21 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 10 | 0.21 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 2 | 0.21 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 2 | 0.21 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 13 | 0.21 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 13 | 0.21 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 13 | 0.21 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 13 | 0.21 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 13 | 0.21 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 13 | 0.21 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE2 | 9 | 0.21 |
| (1,3936) | 1:189:A:VAL:HA | 1:190:A:LYS:HE3 | 9 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 16 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 16 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 16 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 16 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 16 | 0.21 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 16 | 0.21 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD11 | 1 | 0.21 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD12 | 1 | 0.21 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD13 | 1 | 0.21 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD21 | 1 | 0.21 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD22 | 1 | 0.21 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD23 | 1 | 0.21 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD11 | 1 | 0.21 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD12 | 1 | 0.21 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD13 | 1 | 0.21 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD21 | 1 | 0.21 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD22 | 1 | 0.21 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD23 | 1 | 0.21 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 3 | 0.21 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 3 | 0.21 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 19 | 0.21 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 19 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 17 | 0.21 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 17 | 0.21 |
| (1,3716) | 1:105:A:ASP:HB2 | 1:125:A:TRP:HA | 5 | 0.21 |
| (1,3716) | 1:105:A:ASP:HB3 | 1:125:A:TRP:HA | 5 | 0.21 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 7 | 0.21 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 7 | 0.21 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 7 | 0.21 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 7 | 0.21 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 7 | 0.21 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 7 | 0.21 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB1 | 11 | 0.21 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB2 | 11 | 0.21 |
| (1,3604) | 1:77:A:GLN:HE21 | 1:126:A:ALA:HB3 | 11 | 0.21 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB1 | 11 | 0.21 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB2 | 11 | 0.21 |
| (1,3604) | 1:77:A:GLN:HE22 | 1:126:A:ALA:HB3 | 11 | 0.21 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 9 | 0.21 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 9 | 0.21 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 9 | 0.21 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 9 | 0.21 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 9 | 0.21 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 9 | 0.21 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 16 | 0.21 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 16 | 0.21 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 16 | 0.21 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 16 | 0.21 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD21 | 4 | 0.21 |
| (1,3551) | 1:54:A:ILE:HA | 1:55:A:ASN:HD22 | 4 | 0.21 |
| (1,3538) | 1:48:A:ASN:HD21 | 1:49:A:ASP:H | 18 | 0.21 |
| (1,3538) | 1:48:A:ASN:HD22 | 1:49:A:ASP:H | 18 | 0.21 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG21 | 9 | 0.21 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG22 | 9 | 0.21 |
| (1,3516) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG23 | 9 | 0.21 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG21 | 9 | 0.21 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG22 | 9 | 0.21 |
| (1,3516) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG23 | 9 | 0.21 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 1 | 0.21 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 1 | 0.21 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 10 | 0.21 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 10 | 0.21 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 10 | 0.21 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 10 | 0.21 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 10 | 0.21 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 7 | 0.21 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 7 | 0.21 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 7 | 0.21 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 15 | 0.21 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 15 | 0.21 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 15 | 0.21 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 18 | 0.21 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 18 | 0.21 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 18 | 0.21 |
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 5 | 0.21 |
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 5 | 0.21 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 5 | 0.21 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 17 | 0.21 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 17 | 0.21 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 17 | 0.21 |
| (1,3386) | 2:8:B:ILE:HD11 | 2:9:B:ILE:H | 10 | 0.21 |
| (1,3386) | 2:8:B:ILE:HD12 | 2:9:B:ILE:H | 10 | 0.21 |
| (1,3386) | 2:8:B:ILE:HD13 | 2:9:B:ILE:H | 10 | 0.21 |
| (1,3353) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG3 | 8 | 0.21 |
| (1,3353) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG3 | 8 | 0.21 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 4 | 0.21 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 19 | 0.21 |
| (1,3277) | 1:69:A:PHE:HD1 | 1:87:A:VAL:HB | 1 | 0.21 |
| (1,3277) | 1:69:A:PHE:HD2 | 1:87:A:VAL:HB | 1 | 0.21 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 3 | 0.21 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 20 | 0.21 |
| (1,3248) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HE1 | 2 | 0.21 |
| (1,3248) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HE1 | 2 | 0.21 |
| (1,3248) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HE1 | 2 | 0.21 |
| (1,3243) | 1:182:A:HIS:HD2 | 1:187:A:MET:HG2 | 9 | 0.21 |
| (1,3228) | 1:125:A:TRP:HE3 | 1:134:A:VAL:HG11 | 16 | 0.21 |
| (1,3228) | 1:125:A:TRP:HE3 | 1:134:A:VAL:HG12 | 16 | 0.21 |
| (1,3228) | 1:125:A:TRP:HE3 | 1:134:A:VAL:HG13 | 16 | 0.21 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 2 | 0.21 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 2 | 0.21 |
| (1,3201) | 1:170:A:PHE:HZ | 1:194:A:ILE:HG13 | 8 | 0.21 |
| (1,3172) | 1:140:A:ILE:HB | 1:165:A:PHE:HZ | 10 | 0.21 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 5 | 0.21 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 5 | 0.21 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 5 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 5 | 0.21 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 5 | 0.21 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 5 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 6 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 6 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 6 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 6 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 6 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 6 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 18 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 18 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 18 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 18 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 18 | 0.21 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 18 | 0.21 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 17 | 0.21 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 17 | 0.21 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 7 | 0.21 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 5 | 0.21 |
| (1,3071) | 1:196:A:ASN:HD21 | 1:225:A:LYS:HB3 | 12 | 0.21 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 14 | 0.21 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 3 | 0.21 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 3 | 0.21 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 3 | 0.21 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 3 | 0.21 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 3 | 0.21 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 14 | 0.21 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 14 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 1 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 2 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 5 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 6 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 8 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 9 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 11 | 0.21 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 17 | 0.21 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 7 | 0.21 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 7 | 0.21 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 7 | 0.21 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 20 | 0.21 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 20 | 0.21 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 20 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2877) | 1:116:A:GLN:HE21 | 1:187:A:MET:H | 3 | 0.21 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 18 | 0.21 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 19 | 0.21 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 19 | 0.21 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 3 | 0.21 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 5 | 0.21 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 10 | 0.21 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 4 | 0.21 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 10 | 0.21 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 16 | 0.21 |
| (1,2820) | 1:174:A:GLU:HB3 | 1:176:A:ALA:H | 17 | 0.21 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 12 | 0.21 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 12 | 0.21 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 12 | 0.21 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 11 | 0.21 |
| (1,2764) | 1:168:A:ALA:H | 1:196:A:ASN:HB2 | 11 | 0.21 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 19 | 0.21 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 5 | 0.21 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 19 | 0.21 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 6 | 0.21 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 6 | 0.21 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 6 | 0.21 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 19 | 0.21 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 2 | 0.21 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 6 | 0.21 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 3 | 0.21 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 3 | 0.21 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 3 | 0.21 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 20 | 0.21 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 20 | 0.21 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 20 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 2 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 2 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 4 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 4 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 9 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 9 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 11 | 0.21 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 11 | 0.21 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 10 | 0.21 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 19 | 0.21 |
| (1,2512) | 1:124:A:GLY:H | 1:136:A:TYR:HB2 | 7 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 19 | 0.21 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 19 | 0.21 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 19 | 0.21 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 2 | 0.21 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 3 | 0.21 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 8 | 0.21 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 9 | 0.21 |
| (1,2466) | 1:118:A:ILE:H | 1:140:A:ILE:HA | 16 | 0.21 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 8 | 0.21 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 8 | 0.21 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG11 | 20 | 0.21 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG12 | 20 | 0.21 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG13 | 20 | 0.21 |
| (1,2381) | 1:98:A:PRO:HG2 | 1:99:A:GLU:H | 11 | 0.21 |
| (1,2381) | 1:98:A:PRO:HG3 | 1:99:A:GLU:H | 11 | 0.21 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 3 | 0.21 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 5 | 0.21 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 6 | 0.21 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 17 | 0.21 |
| (1,2365) | 1:156:A:SER:HA | 1:164:A:GLU:H | 3 | 0.21 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG11 | 20 | 0.21 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG12 | 20 | 0.21 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG13 | 20 | 0.21 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 9 | 0.21 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 12 | 0.21 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 15 | 0.21 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 15 | 0.21 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 16 | 0.21 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 16 | 0.21 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 11 | 0.21 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 14 | 0.21 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 14 | 0.21 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 9 | 0.21 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 2 | 0.21 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 8 | 0.21 |
| (1,2211) | 1:60:A:LYS:H | 1:60:A:LYS:HE3 | 17 | 0.21 |
| (1,2194) | 1:58:A:HIS:H | 1:71:A:GLY:HA2 | 7 | 0.21 |
| (1,2129) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB3 | 11 | 0.21 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE1 | 17 | 0.21 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE2 | 17 | 0.21 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 19 | 0.21 |
| (1,2103) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 19 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 1 | 0.21 |
| (1,2074) | 1:223:A:THR:HB | 1:224:A:LEU:H | 11 | 0.21 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 7 | 0.21 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 7 | 0.21 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 7 | 0.21 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 4 | 0.21 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 4 | 0.21 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 4 | 0.21 |
| (1,2002) | 1:216:A:LEU:H | 1:216:A:LEU:HG | 13 | 0.21 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 7 | 0.21 |
| (1,1997) | 1:184:A:ILE:HA | 1:216:A:LEU:HB3 | 4 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 3 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 8 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 13 | 0.21 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 13 | 0.21 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 2 | 0.21 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 5 | 0.21 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 6 | 0.21 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 14 | 0.21 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 15 | 0.21 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 2 | 0.21 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 2 | 0.21 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 2 | 0.21 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 18 | 0.21 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 18 | 0.21 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 18 | 0.21 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 3 | 0.21 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 3 | 0.21 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 2 | 0.21 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 7 | 0.21 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 20 | 0.21 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD2 | 2 | 0.21 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD3 | 2 | 0.21 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD2 | 2 | 0.21 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD3 | 2 | 0.21 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD2 | 2 | 0.21 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD3 | 2 | 0.21 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 14 | 0.21 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 13 | 0.21 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 13 | 0.21 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 13 | 0.21 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 1 | 0.21 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 7 | 0.21 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 20 | 0.21 |
| (1,1707) | 1:194:A:ILE:HG21 | 1:196:A:ASN:HA | 9 | 0.21 |
| (1,1707) | 1:194:A:ILE:HG22 | 1:196:A:ASN:HA | 9 | 0.21 |
| (1,1707) | 1:194:A:ILE:HG23 | 1:196:A:ASN:HA | 9 | 0.21 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 7 | 0.21 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 7 | 0.21 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 7 | 0.21 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 1 | 0.21 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 1 | 0.21 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 1 | 0.21 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 2 | 0.21 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 2 | 0.21 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 2 | 0.21 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 14 | 0.21 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 14 | 0.21 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 14 | 0.21 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 19 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 5 | 0.21 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 12 | 0.21 |
| (1,1554) | 1:184:A:ILE:HD11 | 1:190:A:LYS:HA | 16 | 0.21 |
| (1,1554) | 1:184:A:ILE:HD12 | 1:190:A:LYS:HA | 16 | 0.21 |
| (1,1554) | 1:184:A:ILE:HD13 | 1:190:A:LYS:HA | 16 | 0.21 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 3 | 0.21 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 3 | 0.21 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 3 | 0.21 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 11 | 0.21 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 11 | 0.21 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 11 | 0.21 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 15 | 0.21 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 15 | 0.21 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 15 | 0.21 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 19 | 0.21 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 19 | 0.21 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 19 | 0.21 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 7 | 0.21 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 7 | 0.21 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 7 | 0.21 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD11 | 9 | 0.21 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD12 | 9 | 0.21 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD13 | 9 | 0.21 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD21 | 9 | 0.21 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD22 | 9 | 0.21 |
| (1,1476) | 1:147:A:GLY:HA2 | 1:179:A:LEU:HD23 | 9 | 0.21 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 15 | 0.21 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 15 | 0.21 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 15 | 0.21 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 1 | 0.21 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 4 | 0.21 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 9 | 0.21 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 13 | 0.21 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 17 | 0.21 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD11 | 3 | 0.21 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD12 | 3 | 0.21 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD13 | 3 | 0.21 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD21 | 3 | 0.21 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD22 | 3 | 0.21 |
| (1,1442) | 1:178:A:ALA:HA | 1:179:A:LEU:HD23 | 3 | 0.21 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 13 | 0.21 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 13 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 13 | 0.21 |
| (1,1397) | 1:174:A:GLU:HA | 1:177:A:GLU:HA | 1 | 0.21 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 8 | 0.21 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 13 | 0.21 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 15 | 0.21 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 1 | 0.21 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 11 | 0.21 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 11 | 0.21 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 11 | 0.21 |
| (1,1363) | 1:153:A:VAL:H | 1:166:A:ASP:HB2 | 12 | 0.21 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 14 | 0.21 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD11 | 3 | 0.21 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD12 | 3 | 0.21 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD13 | 3 | 0.21 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD21 | 3 | 0.21 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD22 | 3 | 0.21 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD23 | 3 | 0.21 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 16 | 0.21 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 16 | 0.21 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 16 | 0.21 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 16 | 0.21 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 4 | 0.21 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 4 | 0.21 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 4 | 0.21 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 16 | 0.21 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 16 | 0.21 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 16 | 0.21 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 9 | 0.21 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 2 | 0.21 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 2 | 0.21 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 2 | 0.21 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 8 | 0.21 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 8 | 0.21 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 8 | 0.21 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD2 | 2 | 0.21 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD3 | 2 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB1 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB2 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB3 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB1 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB2 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB3 | 11 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB1 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB2 | 11 | 0.21 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB3 | 11 | 0.21 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 15 | 0.21 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 15 | 0.21 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 5 | 0.21 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 5 | 0.21 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 15 | 0.21 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 15 | 0.21 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 16 | 0.21 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 16 | 0.21 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 16 | 0.21 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 16 | 0.21 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 16 | 0.21 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 8 | 0.21 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 8 | 0.21 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 8 | 0.21 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 17 | 0.21 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 17 | 0.21 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 17 | 0.21 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 5 | 0.21 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 5 | 0.21 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 5 | 0.21 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 5 | 0.21 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 5 | 0.21 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 5 | 0.21 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 3 | 0.21 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 8 | 0.21 |
| (1,1054) | 1:139:A:SER:HB2 | 1:149:A:ALA:H | 12 | 0.21 |
| (1,1053) | 1:139:A:SER:HB3 | 1:140:A:ILE:H | 18 | 0.21 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 18 | 0.21 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 18 | 0.21 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 18 | 0.21 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 9 | 0.21 |
| (1,1002) | 1:123:A:LYS:HD3 | 1:136:A:TYR:HB3 | 12 | 0.21 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 1 | 0.21 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 1 | 0.21 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 5 | 0.21 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 5 | 0.21 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 7 | 0.21 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 7 | 0.21 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 17 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 18 | 0.21 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 6 | 0.21 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 6 | 0.21 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 6 | 0.21 |
| (1,844) | 1:81:A:ARG:HG2 | 1:83:A:GLN:HG3 | 10 | 0.21 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 1 | 0.21 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 1 | 0.21 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 1 | 0.21 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 1 | 0.21 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 1 | 0.21 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 1 | 0.21 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 8 | 0.21 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 8 | 0.21 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 8 | 0.21 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 13 | 0.21 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 19 | 0.21 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 19 | 0.21 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 11 | 0.21 |
| (1,769) | 1:82:A:LEU:HG | 1:112:A:TYR:HA | 18 | 0.21 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 2 | 0.21 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 15 | 0.21 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 11 | 0.21 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 7 | 0.21 |
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 7 | 0.21 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG21 | 9 | 0.21 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG22 | 9 | 0.21 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG23 | 9 | 0.21 |
| (1,653) | 1:102:A:ARG:HD2 | 2:8:B:ILE:HG12 | 5 | 0.21 |
| (1,653) | 1:102:A:ARG:HD3 | 2:8:B:ILE:HG12 | 5 | 0.21 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 19 | 0.21 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 13 | 0.21 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 13 | 0.21 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 13 | 0.21 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 19 | 0.21 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 19 | 0.21 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 20 | 0.21 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 20 | 0.21 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 20 | 0.21 |
| (1,526) | 1:87:A:VAL:HG11 | 1:104:A:VAL:HA | 16 | 0.21 |
| (1,526) | 1:87:A:VAL:HG12 | 1:104:A:VAL:HA | 16 | 0.21 |
| (1,526) | 1:87:A:VAL:HG13 | 1:104:A:VAL:HA | 16 | 0.21 |
| (1,526) | 1:87:A:VAL:HG21 | 1:104:A:VAL:HA | 16 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,526) | 1:87:A:VAL:HG22 | 1:104:A:VAL:HA | 16 | 0.21 |
| (1,526) | 1:87:A:VAL:HG23 | 1:104:A:VAL:HA | 16 | 0.21 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 5 | 0.21 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 12 | 0.21 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 15 | 0.21 |
| (1,521) | 1:86:A:GLU:H | 1:87:A:VAL:HB | 2 | 0.21 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 15 | 0.21 |
| (1,462) | 1:81:A:ARG:HA | 1:81:A:ARG:HD3 | 7 | 0.21 |
| (1,462) | 1:81:A:ARG:HA | 1:81:A:ARG:HD3 | 18 | 0.21 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 5 | 0.21 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 5 | 0.21 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 5 | 0.21 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 16 | 0.21 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 16 | 0.21 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 2 | 0.21 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 2 | 0.21 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 2 | 0.21 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 8 | 0.21 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 8 | 0.21 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 8 | 0.21 |
| (1,280) | 1:68:A:VAL:HB | 1:70:A:THR:HG21 | 6 | 0.21 |
| (1,280) | 1:68:A:VAL:HB | 1:70:A:THR:HG22 | 6 | 0.21 |
| (1,280) | 1:68:A:VAL:HB | 1:70:A:THR:HG23 | 6 | 0.21 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 4 | 0.21 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 4 | 0.21 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 4 | 0.21 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 10 | 0.21 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 10 | 0.21 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 10 | 0.21 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 11 | 0.21 |
| (1,191) | 1:152:A:LYS:H | 1:168:A:ALA:HA | 11 | 0.21 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 3 | 0.21 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 3 | 0.21 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 3 | 0.21 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 16 | 0.21 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 16 | 0.21 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 16 | 0.21 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 12 | 0.21 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 12 | 0.21 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 12 | 0.21 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 17 | 0.21 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 17 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 17 | 0.21 |
| (1,103) | 1:54:A:ILE:HA | 1:54:A:ILE:HG12 | 18 | 0.21 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 19 | 0.21 |
| (1,65) | 1:52:A:VAL:HG11 | 1:76:A:MET:H | 12 | 0.21 |
| (1,65) | 1:52:A:VAL:HG12 | 1:76:A:MET:H | 12 | 0.21 |
| (1,65) | 1:52:A:VAL:HG13 | 1:76:A:MET:H | 12 | 0.21 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE2 | 12 | 0.21 |
| (1,5) | 1:173:A:TYR:HA | 1:205:A:LYS:HE3 | 12 | 0.21 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 7 | 0.2 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 7 | 0.2 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 3 | 0.2 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 3 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 15 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 15 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 15 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 15 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 15 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 15 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 19 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 19 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 19 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 19 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 19 | 0.2 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 19 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB2 | 7 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB3 | 7 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB2 | 7 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB3 | 7 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB2 | 7 | 0.2 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB3 | 7 | 0.2 |
| (1,3965) | 1:204:A:GLU:HG2 | 1:205:A:LYS:HE2 | 17 | 0.2 |
| (1,3965) | 1:204:A:GLU:HG2 | 1:205:A:LYS:HE3 | 17 | 0.2 |
| (1,3965) | 1:204:A:GLU:HG3 | 1:205:A:LYS:HE2 | 17 | 0.2 |
| (1,3965) | 1:204:A:GLU:HG3 | 1:205:A:LYS:HE3 | 17 | 0.2 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 16 | 0.2 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 16 | 0.2 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 16 | 0.2 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 16 | 0.2 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 16 | 0.2 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 16 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 1 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 1 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 1 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 1 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 1 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 7 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 7 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 7 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 7 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 7 | 0.2 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 7 | 0.2 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD11 | 5 | 0.2 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD12 | 5 | 0.2 |
| (1,3928) | 1:185:A:LYS:HE2 | 1:216:A:LEU:HD13 | 5 | 0.2 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD11 | 5 | 0.2 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD12 | 5 | 0.2 |
| (1,3928) | 1:185:A:LYS:HE3 | 1:216:A:LEU:HD13 | 5 | 0.2 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 9 | 0.2 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 9 | 0.2 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 9 | 0.2 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 9 | 0.2 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 9 | 0.2 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 9 | 0.2 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 16 | 0.2 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 16 | 0.2 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 16 | 0.2 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 16 | 0.2 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 16 | 0.2 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 16 | 0.2 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 19 | 0.2 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 19 | 0.2 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 19 | 0.2 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 19 | 0.2 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 19 | 0.2 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 19 | 0.2 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 18 | 0.2 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 18 | 0.2 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 18 | 0.2 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 18 | 0.2 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 18 | 0.2 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 18 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 1 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 7 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 7 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 11 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 11 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 12 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 12 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 17 | 0.2 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 17 | 0.2 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 7 | 0.2 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 7 | 0.2 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE2 | 2 | 0.2 |
| (1,3844) | 1:137:A:ASP:HB3 | 1:152:A:LYS:HE3 | 2 | 0.2 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 1 | 0.2 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 1 | 0.2 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 9 | 0.2 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 9 | 0.2 |
| (1,3687) | 1:96:A:GLY:HA2 | 1:97:A:GLN:HG2 | 1 | 0.2 |
| (1,3687) | 1:96:A:GLY:HA2 | 1:97:A:GLN:HG3 | 1 | 0.2 |
| (1,3687) | 1:96:A:GLY:HA3 | 1:97:A:GLN:HG2 | 1 | 0.2 |
| (1,3687) | 1:96:A:GLY:HA3 | 1:97:A:GLN:HG3 | 1 | 0.2 |
| (1,3617) | 1:80:A:SER:HB2 | 1:115:A:ASN:H | 7 | 0.2 |
| (1,3617) | 1:80:A:SER:HB3 | 1:115:A:ASN:H | 7 | 0.2 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 19 | 0.2 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 19 | 0.2 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 19 | 0.2 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 19 | 0.2 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 8 | 0.2 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 8 | 0.2 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 8 | 0.2 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 6 | 0.2 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 6 | 0.2 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 6 | 0.2 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 17 | 0.2 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 17 | 0.2 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 17 | 0.2 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 17 | 0.2 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 15 | 0.2 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 15 | 0.2 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 15 | 0.2 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 15 | 0.2 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 15 | 0.2 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 15 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 12 | 0.2 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 12 | 0.2 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 12 | 0.2 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 12 | 0.2 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 12 | 0.2 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 12 | 0.2 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 6 | 0.2 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 6 | 0.2 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 6 | 0.2 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 11 | 0.2 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 11 | 0.2 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 11 | 0.2 |
| (1,3479) | 1:53:A:THR:HG21 | 2:9:B:ILE:HB | 10 | 0.2 |
| (1,3479) | 1:53:A:THR:HG22 | 2:9:B:ILE:HB | 10 | 0.2 |
| (1,3479) | 1:53:A:THR:HG23 | 2:9:B:ILE:HB | 10 | 0.2 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 10 | 0.2 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 10 | 0.2 |
| (1,3352) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG2 | 19 | 0.2 |
| (1,3352) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG2 | 19 | 0.2 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 2 | 0.2 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 9 | 0.2 |
| (1,3329) | 2:20:B:ARG:HD2 | 2:21:B:MET:H | 1 | 0.2 |
| (1,3329) | 2:20:B:ARG:HD3 | 2:21:B:MET:H | 1 | 0.2 |
| (1,3326) | 2:21:B:MET:H | 2:21:B:MET:HE1 | 13 | 0.2 |
| (1,3326) | 2:21:B:MET:H | 2:21:B:MET:HE2 | 13 | 0.2 |
| (1,3326) | 2:21:B:MET:H | 2:21:B:MET:HE3 | 13 | 0.2 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 16 | 0.2 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 15 | 0.2 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 4 | 0.2 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 11 | 0.2 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 7 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 8 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 8 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 8 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 8 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 8 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 8 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 10 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 10 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 10 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 10 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 10 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 12 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 12 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 12 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 12 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 12 | 0.2 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 12 | 0.2 |
| (1,3113) | 1:136:A:TYR:HD1 | 1:137:A:ASP:H | 7 | 0.2 |
| (1,3113) | 1:136:A:TYR:HD2 | 1:137:A:ASP:H | 7 | 0.2 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 3 | 0.2 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 10 | 0.2 |
| (1,3019) | 1:216:A:LEU:HB2 | 1:218:A:ALA:H | 17 | 0.2 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 1 | 0.2 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 18 | 0.2 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 14 | 0.2 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 14 | 0.2 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 14 | 0.2 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 19 | 0.2 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 10 | 0.2 |
| (1,2927) | 1:195:A:ASN:HB2 | 1:196:A:ASN:H | 4 | 0.2 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 4 | 0.2 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 18 | 0.2 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 12 | 0.2 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 17 | 0.2 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 17 | 0.2 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 17 | 0.2 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 4 | 0.2 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 11 | 0.2 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 8 | 0.2 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 8 | 0.2 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 8 | 0.2 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 16 | 0.2 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 16 | 0.2 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 16 | 0.2 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 14 | 0.2 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 20 | 0.2 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 3 | 0.2 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 3 | 0.2 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 3 | 0.2 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 3 | 0.2 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 3 | 0.2 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 17 | 0.2 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 6 | 0.2 |
| (1,2652) | 1:149:A:ALA:H | 1:179:A:LEU:HB3 | 3 | 0.2 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 2 | 0.2 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 3 | 0.2 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 16 | 0.2 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 11 | 0.2 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 4 | 0.2 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 4 | 0.2 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 4 | 0.2 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 17 | 0.2 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 17 | 0.2 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 17 | 0.2 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 1 | 0.2 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 1 | 0.2 |
| (1,2579) | 1:215:A:GLU:HB2 | 1:216:A:LEU:H | 18 | 0.2 |
| (1,2579) | 1:215:A:GLU:HB3 | 1:216:A:LEU:H | 18 | 0.2 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 12 | 0.2 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 4 | 0.2 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 4 | 0.2 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 4 | 0.2 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 10 | 0.2 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 10 | 0.2 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 10 | 0.2 |
| (1,2546) | 1:127:A:ASN:HD21 | 1:132:A:ASP:H | 17 | 0.2 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 12 | 0.2 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 12 | 0.2 |
| (1,2480) | 1:118:A:ILE:HG13 | 1:119:A:LEU:H | 1 | 0.2 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 6 | 0.2 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 12 | 0.2 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 6 | 0.2 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 6 | 0.2 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 6 | 0.2 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 7 | 0.2 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 8 | 0.2 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 13 | 0.2 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG11 | 17 | 0.2 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG12 | 17 | 0.2 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG13 | 17 | 0.2 |
| (1,2303) | 1:77:A:GLN:HB2 | 1:80:A:SER:H | 1 | 0.2 |
| (1,2303) | 1:77:A:GLN:HB2 | 1:80:A:SER:H | 12 | 0.2 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2190) | 1:58:A:HIS:H | 2:12:B:ASN:HD22 | 1 | 0.2 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 5 | 0.2 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 8 | 0.2 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 8 | 0.2 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 8 | 0.2 |
| (1,2129) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB3 | 19 | 0.2 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 4 | 0.2 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 4 | 0.2 |
| (1,2094) | 1:50:A:LEU:H | 1:50:A:LEU:HG | 13 | 0.2 |
| (1,2074) | 1:223:A:THR:HB | 1:224:A:LEU:H | 12 | 0.2 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 16 | 0.2 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 16 | 0.2 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 16 | 0.2 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 7 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 9 | 0.2 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 9 | 0.2 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 12 | 0.2 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 2 | 0.2 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 2 | 0.2 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 5 | 0.2 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 5 | 0.2 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 18 | 0.2 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 5 | 0.2 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 5 | 0.2 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 5 | 0.2 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD2 | 13 | 0.2 |
| (1,1829) | 1:207:A:THR:HG21 | 1:210:A:LYS:HD3 | 13 | 0.2 |
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD2 | 13 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1829) | 1:207:A:THR:HG22 | 1:210:A:LYS:HD3 | 13 | 0.2 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD2 | 13 | 0.2 |
| (1,1829) | 1:207:A:THR:HG23 | 1:210:A:LYS:HD3 | 13 | 0.2 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 5 | 0.2 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 19 | 0.2 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 9 | 0.2 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 7 | 0.2 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 7 | 0.2 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 7 | 0.2 |
| (1,1676) | 1:164:A:GLU:HG2 | 1:193:A:THR:HB | 7 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 3 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 3 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 3 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 18 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 18 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 18 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 20 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 20 | 0.2 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 20 | 0.2 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 4 | 0.2 |
| (1,1582) | 1:201:A:ILE:HG21 | 1:205:A:LYS:HB3 | 14 | 0.2 |
| (1,1582) | 1:201:A:ILE:HG22 | 1:205:A:LYS:HB3 | 14 | 0.2 |
| (1,1582) | 1:201:A:ILE:HG23 | 1:205:A:LYS:HB3 | 14 | 0.2 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 9 | 0.2 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 13 | 0.2 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 13 | 0.2 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 13 | 0.2 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 12 | 0.2 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 12 | 0.2 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 12 | 0.2 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 13 | 0.2 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 13 | 0.2 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 13 | 0.2 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 18 | 0.2 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 18 | 0.2 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 18 | 0.2 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 9 | 0.2 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 9 | 0.2 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 9 | 0.2 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 1 | 0.2 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 4 | 0.2 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 18 | 0.2 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 20 | 0.2 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 20 | 0.2 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 20 | 0.2 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 20 | 0.2 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 20 | 0.2 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 20 | 0.2 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 13 | 0.2 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 3 | 0.2 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 16 | 0.2 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 10 | 0.2 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 10 | 0.2 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 10 | 0.2 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 17 | 0.2 |
| (1,1380) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB2 | 17 | 0.2 |
| (1,1380) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB2 | 17 | 0.2 |
| (1,1380) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB2 | 17 | 0.2 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 2 | 0.2 |
| (1,1368) | 1:63:A:TYR:HB2 | 1:67:A:ALA:H | 9 | 0.2 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 20 | 0.2 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 20 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 15 | 0.2 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 15 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 1 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 1 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 1 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 18 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 18 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 18 | 0.2 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 18 | 0.2 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 17 | 0.2 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG21 | 13 | 0.2 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG22 | 13 | 0.2 |
| (1,1234) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HG23 | 13 | 0.2 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 7 | 0.2 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 7 | 0.2 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 7 | 0.2 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 14 | 0.2 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 14 | 0.2 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 14 | 0.2 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD2 | 8 | 0.2 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD3 | 8 | 0.2 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 18 | 0.2 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 18 | 0.2 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 18 | 0.2 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 7 | 0.2 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 14 | 0.2 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 14 | 0.2 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 14 | 0.2 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 18 | 0.2 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 18 | 0.2 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 18 | 0.2 |
| (1,1146) | 1:142:A:THR:HA | 1:147:A:GLY:HA3 | 18 | 0.2 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 9 | 0.2 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 9 | 0.2 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 9 | 0.2 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 9 | 0.2 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 9 | 0.2 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 9 | 0.2 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 9 | 0.2 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 9 | 0.2 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 9 | 0.2 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 4 | 0.2 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 4 | 0.2 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 4 | 0.2 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 13 | 0.2 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 13 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 13 | 0.2 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 12 | 0.2 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 12 | 0.2 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 12 | 0.2 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 16 | 0.2 |
| (1,976) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HB3 | 16 | 0.2 |
| (1,976) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HB3 | 16 | 0.2 |
| (1,976) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HB3 | 16 | 0.2 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB1 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB2 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB3 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB1 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB2 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB3 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB1 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB2 | 9 | 0.2 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB3 | 9 | 0.2 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB1 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB2 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG21 | 1:67:A:ALA:HB3 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB1 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB2 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG22 | 1:67:A:ALA:HB3 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB1 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB2 | 12 | 0.2 |
| (1,925) | 1:54:A:ILE:HG23 | 1:67:A:ALA:HB3 | 12 | 0.2 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 15 | 0.2 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 15 | 0.2 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 15 | 0.2 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 3 | 0.2 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 3 | 0.2 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 15 | 0.2 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 15 | 0.2 |
| (1,891) | 1:123:A:LYS:HD2 | 1:124:A:GLY:H | 7 | 0.2 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 7 | 0.2 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 7 | 0.2 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 7 | 0.2 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 14 | 0.2 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 14 | 0.2 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 14 | 0.2 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 16 | 0.2 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 16 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 16 | 0.2 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 20 | 0.2 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 20 | 0.2 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 20 | 0.2 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 7 | 0.2 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 7 | 0.2 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 7 | 0.2 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 18 | 0.2 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 1 | 0.2 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 6 | 0.2 |
| (1,766) | 1:145:A:ALA:HA | 1:182:A:HIS:HB2 | 5 | 0.2 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 18 | 0.2 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 10 | 0.2 |
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 18 | 0.2 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD2 | 12 | 0.2 |
| (1,656) | 1:151:A:ALA:HA | 1:152:A:LYS:HD3 | 12 | 0.2 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 9 | 0.2 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 9 | 0.2 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 12 | 0.2 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD11 | 12 | 0.2 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD12 | 12 | 0.2 |
| (1,611) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HD13 | 12 | 0.2 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD11 | 12 | 0.2 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD12 | 12 | 0.2 |
| (1,611) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HD13 | 12 | 0.2 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 13 | 0.2 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 13 | 0.2 |
| (1,581) | 1:92:A:LYS:HA | 1:92:A:LYS:HG2 | 8 | 0.2 |
| (1,581) | 1:92:A:LYS:HA | 1:92:A:LYS:HG3 | 8 | 0.2 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD2 | 2 | 0.2 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD3 | 2 | 0.2 |
| (1,564) | 1:74:A:ASP:HA | 1:75:A:ILE:HB | 6 | 0.2 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 15 | 0.2 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 3 | 0.2 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 8 | 0.2 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 12 | 0.2 |
| (1,425) | 1:53:A:THR:HG21 | 1:76:A:MET:HG2 | 8 | 0.2 |
| (1,425) | 1:53:A:THR:HG21 | 1:76:A:MET:HG3 | 8 | 0.2 |
| (1,425) | 1:53:A:THR:HG22 | 1:76:A:MET:HG2 | 8 | 0.2 |
| (1,425) | 1:53:A:THR:HG22 | 1:76:A:MET:HG3 | 8 | 0.2 |
| (1,425) | 1:53:A:THR:HG23 | 1:76:A:MET:HG2 | 8 | 0.2 |
| (1,425) | 1:53:A:THR:HG23 | 1:76:A:MET:HG3 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 4 | 0.2 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 4 | 0.2 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 4 | 0.2 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 6 | 0.2 |
| (1,242) | 1:142:A:THR:HG21 | 1:146:A:PRO:HD2 | 20 | 0.2 |
| (1,242) | 1:142:A:THR:HG22 | 1:146:A:PRO:HD2 | 20 | 0.2 |
| (1,242) | 1:142:A:THR:HG23 | 1:146:A:PRO:HD2 | 20 | 0.2 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 7 | 0.2 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 3 | 0.2 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 3 | 0.2 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 3 | 0.2 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 4 | 0.2 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 4 | 0.2 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 4 | 0.2 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 7 | 0.2 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 7 | 0.2 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 7 | 0.2 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 9 | 0.2 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 9 | 0.2 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 9 | 0.2 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 2 | 0.2 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 2 | 0.2 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 2 | 0.2 |
| (1,155) | 1:60:A:LYS:HG2 | 1:60:A:LYS:HE2 | 17 | 0.2 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 11 | 0.2 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 11 | 0.2 |
| (1,101) | 1:53:A:THR:HG21 | 1:55:A:ASN:HD21 | 4 | 0.2 |
| (1,101) | 1:53:A:THR:HG22 | 1:55:A:ASN:HD21 | 4 | 0.2 |
| (1,101) | 1:53:A:THR:HG23 | 1:55:A:ASN:HD21 | 4 | 0.2 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 8 | 0.2 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 8 | 0.2 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 2 | 0.2 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 20 | 0.2 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 8 | 0.2 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 8 | 0.2 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 5 | 0.2 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 20 | 0.2 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 20 | 0.2 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 20 | 0.2 |
| (1,37) | 1:51:A:PRO:HA | 2:7:B:PRO:HD2 | 16 | 0.2 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 1 | 0.2 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 1 | 0.2 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 1 | 0.2 |
| (1,29) | 1:85:A:ASP:H | 1:109:A:ASN:HB3 | 20 | 0.2 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 10 | 0.19 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 10 | 0.19 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 19 | 0.19 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 19 | 0.19 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 8 | 0.19 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 8 | 0.19 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 8 | 0.19 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 8 | 0.19 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 8 | 0.19 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 8 | 0.19 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 20 | 0.19 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 20 | 0.19 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 4 | 0.19 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 4 | 0.19 |
| (1,3753) | 1:112:A:TYR:H | 1:120:A:LYS:HD2 | 7 | 0.19 |
| (1,3753) | 1:112:A:TYR:H | 1:120:A:LYS:HD3 | 7 | 0.19 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD2 | 19 | 0.19 |
| (1,3751) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HD3 | 19 | 0.19 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG21 | 20 | 0.19 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG22 | 20 | 0.19 |
| (1,3705) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG23 | 20 | 0.19 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG21 | 20 | 0.19 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG22 | 20 | 0.19 |
| (1,3705) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG23 | 20 | 0.19 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 19 | 0.19 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 19 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 8 | 0.19 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 8 | 0.19 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE2 | 7 | 0.19 |
| (1,3542) | 1:49:A:ASP:HB2 | 2:4:B:LYS:HE3 | 7 | 0.19 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE2 | 7 | 0.19 |
| (1,3542) | 1:49:A:ASP:HB3 | 2:4:B:LYS:HE3 | 7 | 0.19 |
| (1,3538) | 1:48:A:ASN:HD21 | 1:49:A:ASP:H | 17 | 0.19 |
| (1,3538) | 1:48:A:ASN:HD22 | 1:49:A:ASP:H | 17 | 0.19 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 13 | 0.19 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 13 | 0.19 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 13 | 0.19 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 10 | 0.19 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 10 | 0.19 |
| (1,3496) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HA | 4 | 0.19 |
| (1,3496) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HA | 4 | 0.19 |
| (1,3496) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HA | 4 | 0.19 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 9 | 0.19 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 9 | 0.19 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 9 | 0.19 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 9 | 0.19 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 9 | 0.19 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 9 | 0.19 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 4 | 0.19 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 4 | 0.19 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 4 | 0.19 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 13 | 0.19 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 13 | 0.19 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 13 | 0.19 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 13 | 0.19 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 13 | 0.19 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 13 | 0.19 |
| (1,3405) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HB3 | 12 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3405) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HB3 | 12 | 0.19 |
| (1,3405) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HB3 | 12 | 0.19 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD2 | 13 | 0.19 |
| (1,3404) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HD3 | 13 | 0.19 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD2 | 13 | 0.19 |
| (1,3404) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HD3 | 13 | 0.19 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD2 | 13 | 0.19 |
| (1,3404) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HD3 | 13 | 0.19 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD2 | 3 | 0.19 |
| (1,3403) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HD3 | 3 | 0.19 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD2 | 3 | 0.19 |
| (1,3403) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HD3 | 3 | 0.19 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD2 | 3 | 0.19 |
| (1,3403) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HD3 | 3 | 0.19 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 10 | 0.19 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 19 | 0.19 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 15 | 0.19 |
| (1,3251) | 1:142:A:THR:HB | 1:182:A:HIS:HE1 | 10 | 0.19 |
| (1,3245) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HD2 | 9 | 0.19 |
| (1,3245) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HD2 | 9 | 0.19 |
| (1,3245) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HD2 | 9 | 0.19 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD1 | 12 | 0.19 |
| (1,3214) | 1:133:A:TRP:HZ2 | 1:135:A:PHE:HD2 | 12 | 0.19 |
| (1,3204) | 1:88:A:GLN:HB3 | 1:90:A:HIS:HE1 | 7 | 0.19 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 13 | 0.19 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 13 | 0.19 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 17 | 0.19 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 17 | 0.19 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 12 | 0.19 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 12 | 0.19 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 12 | 0.19 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 16 | 0.19 |
| (1,3091) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 17 | 0.19 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 8 | 0.19 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 18 | 0.19 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 16 | 0.19 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 16 | 0.19 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG21 | 18 | 0.19 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG22 | 18 | 0.19 |
| (1,3059) | 1:115:A:ASN:HD21 | 1:143:A:VAL:HG23 | 18 | 0.19 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 19 | 0.19 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 18 | 0.19 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 4 | 0.19 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 8 | 0.19 |
| (1,3012) | 1:216:A:LEU:HB2 | 1:217:A:GLY:H | 3 | 0.19 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 4 | 0.19 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 6 | 0.19 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 7 | 0.19 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 14 | 0.19 |
| (1,2950) | 1:198:A:THR:HA | 1:199:A:GLY:H | 6 | 0.19 |
| (1,2925) | 1:196:A:ASN:H | 1:225:A:LYS:H | 14 | 0.19 |
| (1,2920) | 1:166:A:ASP:HA | 1:195:A:ASN:H | 10 | 0.19 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 14 | 0.19 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 17 | 0.19 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 1 | 0.19 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 4 | 0.19 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 9 | 0.19 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 16 | 0.19 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 9 | 0.19 |
| (1,2789) | 1:170:A:PHE:HA | 1:172:A:SER:H | 12 | 0.19 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 3 | 0.19 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 20 | 0.19 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 20 | 0.19 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 20 | 0.19 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 20 | 0.19 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 20 | 0.19 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 20 | 0.19 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 14 | 0.19 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 20 | 0.19 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 7 | 0.19 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 1 | 0.19 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 4 | 0.19 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 13 | 0.19 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 9 | 0.19 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 9 | 0.19 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 9 | 0.19 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 12 | 0.19 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 11 | 0.19 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 11 | 0.19 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 11 | 0.19 |
| (1,2555) | 1:123:A:LYS:HB3 | 1:136:A:TYR:H | 19 | 0.19 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 9 | 0.19 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 4 | 0.19 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 4 | 0.19 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 16 | 0.19 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 18 | 0.19 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 20 | 0.19 |
| (1,2362) | 1:164:A:GLU:H | 1:165:A:PHE:HE1 | 13 | 0.19 |
| (1,2362) | 1:164:A:GLU:H | 1:165:A:PHE:HE2 | 13 | 0.19 |
| (1,2322) | 1:73:A:VAL:HG11 | 1:84:A:ALA:H | 5 | 0.19 |
| (1,2322) | 1:73:A:VAL:HG12 | 1:84:A:ALA:H | 5 | 0.19 |
| (1,2322) | 1:73:A:VAL:HG13 | 1:84:A:ALA:H | 5 | 0.19 |
| (1,2319) | 1:74:A:ASP:HA | 1:84:A:ALA:H | 15 | 0.19 |
| (1,2279) | 1:75:A:ILE:H | 1:84:A:ALA:H | 7 | 0.19 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 15 | 0.19 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 17 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD11 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD12 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD13 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD11 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD12 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD13 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD11 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD12 | 16 | 0.19 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD13 | 16 | 0.19 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 1 | 0.19 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 1 | 0.19 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 15 | 0.19 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 2 | 0.19 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 11 | 0.19 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 13 | 0.19 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 8 | 0.19 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 9 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 1 | 0.19 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 1 | 0.19 |
| (1,1795) | 1:201:A:ILE:HD11 | 1:202:A:THR:H | 19 | 0.19 |
| (1,1795) | 1:201:A:ILE:HD12 | 1:202:A:THR:H | 19 | 0.19 |
| (1,1795) | 1:201:A:ILE:HD13 | 1:202:A:THR:H | 19 | 0.19 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 9 | 0.19 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 9 | 0.19 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 9 | 0.19 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 12 | 0.19 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 12 | 0.19 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 12 | 0.19 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 16 | 0.19 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 16 | 0.19 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 16 | 0.19 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 18 | 0.19 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 15 | 0.19 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 17 | 0.19 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 4 | 0.19 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 4 | 0.19 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 4 | 0.19 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 1 | 0.19 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 1 | 0.19 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 1 | 0.19 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 9 | 0.19 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 19 | 0.19 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 19 | 0.19 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 19 | 0.19 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG21 | 3 | 0.19 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG22 | 3 | 0.19 |
| (1,1606) | 1:116:A:GLN:HE21 | 1:186:A:THR:HG23 | 3 | 0.19 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 5 | 0.19 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 5 | 0.19 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 5 | 0.19 |
| (1,1585) | 1:190:A:LYS:HA | 1:190:A:LYS:HE2 | 12 | 0.19 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 4 | 0.19 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 7 | 0.19 |
| (1,1542) | 1:184:A:ILE:HA | 1:189:A:VAL:HB | 9 | 0.19 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 13 | 0.19 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 13 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 15 | 0.19 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 15 | 0.19 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 2 | 0.19 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 16 | 0.19 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 16 | 0.19 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 16 | 0.19 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 10 | 0.19 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 11 | 0.19 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 14 | 0.19 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 16 | 0.19 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 19 | 0.19 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 11 | 0.19 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 17 | 0.19 |
| (1,1443) | 1:177:A:GLU:HB3 | 1:178:A:ALA:HA | 11 | 0.19 |
| (1,1377) | 1:170:A:PHE:HA | 1:199:A:GLY:HA3 | 9 | 0.19 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 5 | 0.19 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 18 | 0.19 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 1 | 0.19 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 15 | 0.19 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 5 | 0.19 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 6 | 0.19 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 7 | 0.19 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 5 | 0.19 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 5 | 0.19 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 5 | 0.19 |
| (1,1111) | 1:116:A:GLN:HA | 1:142:A:THR:HA | 9 | 0.19 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 11 | 0.19 |
| (1,1043) | 1:139:A:SER:HB3 | 1:154:A:ILE:HD11 | 19 | 0.19 |
| (1,1043) | 1:139:A:SER:HB3 | 1:154:A:ILE:HD12 | 19 | 0.19 |
| (1,1043) | 1:139:A:SER:HB3 | 1:154:A:ILE:HD13 | 19 | 0.19 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 9 | 0.19 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 12 | 0.19 |
| (1,990) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HB | 18 | 0.19 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG11 | 2 | 0.19 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG12 | 2 | 0.19 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG13 | 2 | 0.19 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 6 | 0.19 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 1 | 0.19 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 2 | 0.19 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 2 | 0.19 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 2 | 0.19 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 19 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 19 | 0.19 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 19 | 0.19 |
| (1,893) | 1:155:A:LYS:HE3 | 1:166:A:ASP:H | 3 | 0.19 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 8 | 0.19 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 8 | 0.19 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 19 | 0.19 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD21 | 18 | 0.19 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD22 | 18 | 0.19 |
| (1,858) | 1:155:A:LYS:HB3 | 1:157:A:LEU:HD23 | 18 | 0.19 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 19 | 0.19 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 19 | 0.19 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 19 | 0.19 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 5 | 0.19 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 5 | 0.19 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 5 | 0.19 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 14 | 0.19 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 5 | 0.19 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 5 | 0.19 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 17 | 0.19 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 4 | 0.19 |
| (1,651) | 1:102:A:ARG:HA | 1:102:A:ARG:HG3 | 6 | 0.19 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 5 | 0.19 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 5 | 0.19 |
| (1,551) | 1:59:A:ALA:HB1 | 1:69:A:PHE:HE1 | 19 | 0.19 |
| (1,551) | 1:59:A:ALA:HB1 | 1:69:A:PHE:HE2 | 19 | 0.19 |
| (1,551) | 1:59:A:ALA:HB2 | 1:69:A:PHE:HE1 | 19 | 0.19 |
| (1,551) | 1:59:A:ALA:HB2 | 1:69:A:PHE:HE2 | 19 | 0.19 |
| (1,551) | 1:59:A:ALA:HB3 | 1:69:A:PHE:HE1 | 19 | 0.19 |
| (1,551) | 1:59:A:ALA:HB3 | 1:69:A:PHE:HE2 | 19 | 0.19 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD11 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD12 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD13 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD21 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD22 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG21 | 1:163:A:LEU:HD23 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD11 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD12 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD13 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD21 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD22 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG22 | 1:163:A:LEU:HD23 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD11 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD12 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD13 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD21 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD22 | 5 | 0.19 |
| (1,549) | 1:154:A:ILE:HG23 | 1:163:A:LEU:HD23 | 5 | 0.19 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 6 | 0.19 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 9 | 0.19 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 6 | 0.19 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 20 | 0.19 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 2 | 0.19 |
| (1,514) | 1:123:A:LYS:HB3 | 1:136:A:TYR:HB2 | 10 | 0.19 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 17 | 0.19 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 15 | 0.19 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 9 | 0.19 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 9 | 0.19 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 9 | 0.19 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 12 | 0.19 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 12 | 0.19 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 12 | 0.19 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 13 | 0.19 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 13 | 0.19 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 13 | 0.19 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 15 | 0.19 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 15 | 0.19 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 15 | 0.19 |
| (1,388) | 1:75:A:ILE:HD11 | 1:76:A:MET:H | 10 | 0.19 |
| (1,388) | 1:75:A:ILE:HD12 | 1:76:A:MET:H | 10 | 0.19 |
| (1,388) | 1:75:A:ILE:HD13 | 1:76:A:MET:H | 10 | 0.19 |
| (1,363) | 1:71:A:GLY:HA2 | 1:73:A:VAL:HG21 | 15 | 0.19 |
| (1,363) | 1:71:A:GLY:HA2 | 1:73:A:VAL:HG22 | 15 | 0.19 |
| (1,363) | 1:71:A:GLY:HA2 | 1:73:A:VAL:HG23 | 15 | 0.19 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 4 | 0.19 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 4 | 0.19 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 4 | 0.19 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 4 | 0.19 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 4 | 0.19 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 4 | 0.19 |
| (1,320) | 1:58:A:HIS:HB3 | 1:71:A:GLY:HA3 | 7 | 0.19 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 3 | 0.19 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 3 | 0.19 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 3 | 0.19 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 10 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 5 | 0.19 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 5 | 0.19 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 5 | 0.19 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 16 | 0.19 |
| (1,183) | 1:58:A:HIS:HB3 | 2:12:B:ASN:HD22 | 17 | 0.19 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 9 | 0.19 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 9 | 0.19 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 9 | 0.19 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 4 | 0.19 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 4 | 0.19 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 4 | 0.19 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 1 | 0.19 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 1 | 0.19 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 4 | 0.19 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 4 | 0.19 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 17 | 0.19 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 17 | 0.19 |
| (1,105) | 1:54:A:ILE:HB | 2:9:B:ILE:H | 20 | 0.19 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 4 | 0.19 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 18 | 0.19 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 15 | 0.19 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 3 | 0.19 |
| (1,13) | 1:47:A:THR:HB | 1:50:A:LEU:HA | 8 | 0.19 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 1 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 1 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 12 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 12 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 16 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 16 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 18 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 18 | 0.18 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG2 | 16 | 0.18 |
| (1,4020) | 2:12:B:ASN:HD22 | 2:14:B:ARG:HG3 | 16 | 0.18 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 9 | 0.18 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 9 | 0.18 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 9 | 0.18 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 9 | 0.18 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 9 | 0.18 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 9 | 0.18 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB2 | 20 | 0.18 |
| (1,4006) | 2:9:B:ILE:HG21 | 2:20:B:ARG:HB3 | 20 | 0.18 |
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB2 | 20 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4006) | 2:9:B:ILE:HG22 | 2:20:B:ARG:HB3 | 20 | 0.18 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB2 | 20 | 0.18 |
| (1,4006) | 2:9:B:ILE:HG23 | 2:20:B:ARG:HB3 | 20 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 9 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 9 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 9 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 9 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 9 | 0.18 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 9 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 5 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 5 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 5 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 5 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 5 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 5 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 9 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 9 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 9 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 9 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 9 | 0.18 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 9 | 0.18 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 13 | 0.18 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 13 | 0.18 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB2 | 16 | 0.18 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB3 | 16 | 0.18 |
| (1,3766) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG21 | 5 | 0.18 |
| (1,3766) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG22 | 5 | 0.18 |
| (1,3766) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG23 | 5 | 0.18 |
| (1,3766) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG21 | 5 | 0.18 |
| (1,3766) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG22 | 5 | 0.18 |
| (1,3766) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG23 | 5 | 0.18 |
| (1,3716) | 1:105:A:ASP:HB2 | 1:125:A:TRP:HA | 10 | 0.18 |
| (1,3716) | 1:105:A:ASP:HB3 | 1:125:A:TRP:HA | 10 | 0.18 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 2 | 0.18 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 2 | 0.18 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 2 | 0.18 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 2 | 0.18 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB2 | 5 | 0.18 |
| (1,3602) | 1:77:A:GLN:HB3 | 1:80:A:SER:HB3 | 5 | 0.18 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG2 | 19 | 0.18 |
| (1,3568) | 1:63:A:TYR:HE1 | 2:21:B:MET:HG3 | 19 | 0.18 |
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG2 | 19 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,3568) | 1:63:A:TYR:HE2 | 2:21:B:MET:HG3 | 19 | 0.18 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 7 | 0.18 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 7 | 0.18 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 10 | 0.18 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 10 | 0.18 |
| (1,3530) | 1:63:A:TYR:HE1 | 2:21:B:MET:HB2 | 6 | 0.18 |
| (1,3530) | 1:63:A:TYR:HE2 | 2:21:B:MET:HB2 | 6 | 0.18 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 4 | 0.18 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE1 | 15 | 0.18 |
| (1,3494) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HE2 | 15 | 0.18 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE1 | 15 | 0.18 |
| (1,3494) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HE2 | 15 | 0.18 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE1 | 15 | 0.18 |
| (1,3494) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HE2 | 15 | 0.18 |
| (1,3493) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HA | 5 | 0.18 |
| (1,3493) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HA | 5 | 0.18 |
| (1,3493) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HA | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 5 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 11 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 11 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 11 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 11 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 11 | 0.18 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 11 | 0.18 |
| (1,3451) | 2:6:B:VAL:HG21 | 2:8:B:ILE:H | 3 | 0.18 |
| (1,3451) | 2:6:B:VAL:HG22 | 2:8:B:ILE:H | 3 | 0.18 |
| (1,3451) | 2:6:B:VAL:HG23 | 2:8:B:ILE:H | 3 | 0.18 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 15 | 0.18 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 15 | 0.18 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 15 | 0.18 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 15 | 0.18 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 15 | 0.18 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 15 | 0.18 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 9 | 0.18 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 9 | 0.18 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 3 | 0.18 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 3 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 3 | 0.18 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 3 | 0.18 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 9 | 0.18 |
| (1,3289) | 2:4:B:LYS:HB2 | 2:5:B:PRO:HD3 | 19 | 0.18 |
| (1,3289) | 2:4:B:LYS:HB3 | 2:5:B:PRO:HD3 | 19 | 0.18 |
| (1,3249) | 1:143:A:VAL:HB | 1:182:A:HIS:HE1 | 4 | 0.18 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB1 | 10 | 0.18 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB2 | 10 | 0.18 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB3 | 10 | 0.18 |
| (1,3241) | 1:142:A:THR:HB | 1:182:A:HIS:HD2 | 1 | 0.18 |
| (1,3229) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD21 | 12 | 0.18 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB1 | 14 | 0.18 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB2 | 14 | 0.18 |
| (1,3184) | 1:170:A:PHE:HD1 | 1:197:A:ALA:HB3 | 14 | 0.18 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB1 | 14 | 0.18 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB2 | 14 | 0.18 |
| (1,3184) | 1:170:A:PHE:HD2 | 1:197:A:ALA:HB3 | 14 | 0.18 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 7 | 0.18 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 7 | 0.18 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 7 | 0.18 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 7 | 0.18 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 7 | 0.18 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 7 | 0.18 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 8 | 0.18 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 8 | 0.18 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 12 | 0.18 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 12 | 0.18 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 15 | 0.18 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 15 | 0.18 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 16 | 0.18 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 16 | 0.18 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 8 | 0.18 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 8 | 0.18 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 8 | 0.18 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 8 | 0.18 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 8 | 0.18 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 8 | 0.18 |
| (1,3104) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HD1 | 13 | 0.18 |
| (1,3104) | 1:123:A:LYS:HB2 | 1:136:A:TYR:HD2 | 13 | 0.18 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 6 | 0.18 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 9 | 0.18 |
| (1,3064) | 1:195:A:ASN:H | 1:196:A:ASN:HD21 | 12 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 5 | 0.18 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 3 | 0.18 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 14 | 0.18 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 16 | 0.18 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 12 | 0.18 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 12 | 0.18 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 12 | 0.18 |
| (1,3012) | 1:216:A:LEU:HB2 | 1:217:A:GLY:H | 19 | 0.18 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 11 | 0.18 |
| (1,2958) | 1:200:A:ALA:HA | 1:201:A:ILE:H | 3 | 0.18 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 1 | 0.18 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 19 | 0.18 |
| (1,2856) | 1:142:A:THR:HG21 | 1:182:A:HIS:H | 19 | 0.18 |
| (1,2856) | 1:142:A:THR:HG22 | 1:182:A:HIS:H | 19 | 0.18 |
| (1,2856) | 1:142:A:THR:HG23 | 1:182:A:HIS:H | 19 | 0.18 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 3 | 0.18 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 10 | 0.18 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 11 | 0.18 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 11 | 0.18 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 11 | 0.18 |
| (1,2788) | 1:172:A:SER:H | 1:175:A:ASN:H | 10 | 0.18 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 2 | 0.18 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 2 | 0.18 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 2 | 0.18 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG21 | 2 | 0.18 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG22 | 2 | 0.18 |
| (1,2746) | 1:165:A:PHE:H | 1:192:A:ILE:HG23 | 2 | 0.18 |
| (1,2687) | 1:165:A:PHE:H | 1:193:A:THR:H | 12 | 0.18 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 1 | 0.18 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 3 | 0.18 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 9 | 0.18 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 14 | 0.18 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 16 | 0.18 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 18 | 0.18 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 4 | 0.18 |
| (1,2611) | 1:116:A:GLN:H | 1:143:A:VAL:H | 18 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 8 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 8 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 8 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 14 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 14 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 14 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 16 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 16 | 0.18 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 16 | 0.18 |
| (1,2564) | 1:137:A:ASP:H | 1:152:A:LYS:HD2 | 10 | 0.18 |
| (1,2564) | 1:137:A:ASP:H | 1:152:A:LYS:HD3 | 10 | 0.18 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 4 | 0.18 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 4 | 0.18 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 4 | 0.18 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 6 | 0.18 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 3 | 0.18 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 3 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 11 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 11 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 11 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 20 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 20 | 0.18 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 20 | 0.18 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 14 | 0.18 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 14 | 0.18 |
| (1,2393) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 9 | 0.18 |
| (1,2381) | 1:98:A:PRO:HG2 | 1:99:A:GLU:H | 8 | 0.18 |
| (1,2381) | 1:98:A:PRO:HG3 | 1:99:A:GLU:H | 8 | 0.18 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 1 | 0.18 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 15 | 0.18 |
| (1,2372) | 1:92:A:LYS:H | 1:92:A:LYS:HG2 | 9 | 0.18 |
| (1,2372) | 1:92:A:LYS:H | 1:92:A:LYS:HG3 | 9 | 0.18 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 14 | 0.18 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 6 | 0.18 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 18 | 0.18 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 17 | 0.18 |
| (1,2279) | 1:75:A:ILE:H | 1:84:A:ALA:H | 18 | 0.18 |
| (1,2250) | 1:58:A:HIS:HB3 | 1:71:A:GLY:H | 20 | 0.18 |
| (1,2233) | 1:68:A:VAL:H | 1:69:A:PHE:HZ | 5 | 0.18 |
| (1,2178) | 1:56:A:ALA:H | 2:10:B:TYR:HD1 | 19 | 0.18 |
| (1,2178) | 1:56:A:ALA:H | 2:10:B:TYR:HD2 | 19 | 0.18 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG21 | 9 | 0.18 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG22 | 9 | 0.18 |
| (1,2116) | 1:60:A:LYS:H | 1:70:A:THR:HG23 | 9 | 0.18 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 20 | 0.18 |
| (1,2097) | 1:50:A:LEU:HG | 1:51:A:PRO:HD3 | 2 | 0.18 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 17 | 0.18 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 12 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 12 | 0.18 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 12 | 0.18 |
| (1,2031) | 1:191:A:THR:HA | 1:220:A:LEU:HA | 5 | 0.18 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 6 | 0.18 |
| (1,1998) | 1:185:A:LYS:HA | 1:216:A:LEU:HB3 | 10 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB1 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB2 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD11 | 1:214:A:ALA:HB3 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB1 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB2 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD12 | 1:214:A:ALA:HB3 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB1 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB2 | 2 | 0.18 |
| (1,1952) | 1:184:A:ILE:HD13 | 1:214:A:ALA:HB3 | 2 | 0.18 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 17 | 0.18 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 20 | 0.18 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 20 | 0.18 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 20 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 6 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 6 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 7 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 7 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 17 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 17 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 20 | 0.18 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 20 | 0.18 |
| (1,1869) | 1:202:A:THR:H | 1:205:A:LYS:HD3 | 10 | 0.18 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 15 | 0.18 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 17 | 0.18 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 19 | 0.18 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 20 | 0.18 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 20 | 0.18 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 20 | 0.18 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 4 | 0.18 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 6 | 0.18 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 16 | 0.18 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 3 | 0.18 |
| (1,1713) | 1:194:A:ILE:HG21 | 1:195:A:ASN:HA | 11 | 0.18 |
| (1,1713) | 1:194:A:ILE:HG22 | 1:195:A:ASN:HA | 11 | 0.18 |
| (1,1713) | 1:194:A:ILE:HG23 | 1:195:A:ASN:HA | 11 | 0.18 |
| (1,1674) | 1:192:A:ILE:HG21 | 1:193:A:THR:HB | 9 | 0.18 |
| (1,1674) | 1:192:A:ILE:HG22 | 1:193:A:THR:HB | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1674) | 1:192:A:ILE:HG23 | 1:193:A:THR:HB | 9 | 0.18 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD11 | 19 | 0.18 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD12 | 19 | 0.18 |
| (1,1654) | 1:165:A:PHE:HE1 | 1:192:A:ILE:HD13 | 19 | 0.18 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD11 | 19 | 0.18 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD12 | 19 | 0.18 |
| (1,1654) | 1:165:A:PHE:HE2 | 1:192:A:ILE:HD13 | 19 | 0.18 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 10 | 0.18 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 10 | 0.18 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 10 | 0.18 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 6 | 0.18 |
| (1,1567) | 1:184:A:ILE:HG21 | 1:189:A:VAL:H | 1 | 0.18 |
| (1,1567) | 1:184:A:ILE:HG22 | 1:189:A:VAL:H | 1 | 0.18 |
| (1,1567) | 1:184:A:ILE:HG23 | 1:189:A:VAL:H | 1 | 0.18 |
| (1,1562) | 1:184:A:ILE:HG12 | 1:190:A:LYS:H | 13 | 0.18 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 8 | 0.18 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 8 | 0.18 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 8 | 0.18 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 1 | 0.18 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 1 | 0.18 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 1 | 0.18 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 2 | 0.18 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 2 | 0.18 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 2 | 0.18 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 6 | 0.18 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 14 | 0.18 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 16 | 0.18 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 8 | 0.18 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 8 | 0.18 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 8 | 0.18 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 2 | 0.18 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 6 | 0.18 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 7 | 0.18 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 13 | 0.18 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 17 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD11 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD12 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD13 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD11 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD12 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD13 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD11 | 13 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD12 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD13 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD11 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD12 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD13 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD11 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD12 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD13 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD11 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD12 | 13 | 0.18 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD13 | 13 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 7 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 7 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 7 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 7 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 7 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 7 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 12 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 12 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 12 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 12 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 12 | 0.18 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 12 | 0.18 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 2 | 0.18 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 2 | 0.18 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 2 | 0.18 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 16 | 0.18 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 6 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD11 | 2 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD12 | 2 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD13 | 2 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD21 | 2 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD22 | 2 | 0.18 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD23 | 2 | 0.18 |
| (1,1340) | 1:163:A:LEU:HB2 | 1:165:A:PHE:H | 7 | 0.18 |
| (1,1340) | 1:163:A:LEU:HB3 | 1:165:A:PHE:H | 7 | 0.18 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 11 | 0.18 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 11 | 0.18 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 11 | 0.18 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 5 | 0.18 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 19 | 0.18 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 19 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 19 | 0.18 |
| (1,1220) | 1:53:A:THR:HG21 | 1:55:A:ASN:H | 18 | 0.18 |
| (1,1220) | 1:53:A:THR:HG22 | 1:55:A:ASN:H | 18 | 0.18 |
| (1,1220) | 1:53:A:THR:HG23 | 1:55:A:ASN:H | 18 | 0.18 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 5 | 0.18 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 5 | 0.18 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 5 | 0.18 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 17 | 0.18 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 17 | 0.18 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 17 | 0.18 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 12 | 0.18 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 15 | 0.18 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 4 | 0.18 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 4 | 0.18 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 4 | 0.18 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB1 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB2 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG21 | 1:145:A:ALA:HB3 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB1 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB2 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG22 | 1:145:A:ALA:HB3 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB1 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB2 | 10 | 0.18 |
| (1,1134) | 1:142:A:THR:HG23 | 1:145:A:ALA:HB3 | 10 | 0.18 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 5 | 0.18 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 5 | 0.18 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD1 | 5 | 0.18 |
| (1,1092) | 1:140:A:ILE:HG21 | 1:165:A:PHE:HD2 | 5 | 0.18 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD1 | 5 | 0.18 |
| (1,1092) | 1:140:A:ILE:HG22 | 1:165:A:PHE:HD2 | 5 | 0.18 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD1 | 5 | 0.18 |
| (1,1092) | 1:140:A:ILE:HG23 | 1:165:A:PHE:HD2 | 5 | 0.18 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG11 | 1 | 0.18 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG12 | 1 | 0.18 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG13 | 1 | 0.18 |
| (1,976) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HB3 | 1 | 0.18 |
| (1,976) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HB3 | 1 | 0.18 |
| (1,976) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HB3 | 1 | 0.18 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE2 | 14 | 0.18 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE3 | 14 | 0.18 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE2 | 17 | 0.18 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE3 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,950) | 1:130:A:THR:HB | 1:131:A:LYS:H | 16 | 0.18 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 8 | 0.18 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 17 | 0.18 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 17 | 0.18 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 17 | 0.18 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 4 | 0.18 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 4 | 0.18 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 11 | 0.18 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 11 | 0.18 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 12 | 0.18 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 12 | 0.18 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 16 | 0.18 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 16 | 0.18 |
| (1,853) | 1:210:A:LYS:HA | 1:220:A:LEU:HG | 12 | 0.18 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 14 | 0.18 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 14 | 0.18 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 14 | 0.18 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 16 | 0.18 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 16 | 0.18 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 16 | 0.18 |
| (1,815) | 1:117:A:VAL:HG11 | 1:118:A:ILE:HG13 | 3 | 0.18 |
| (1,815) | 1:117:A:VAL:HG12 | 1:118:A:ILE:HG13 | 3 | 0.18 |
| (1,815) | 1:117:A:VAL:HG13 | 1:118:A:ILE:HG13 | 3 | 0.18 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 1 | 0.18 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 9 | 0.18 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 15 | 0.18 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 17 | 0.18 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 13 | 0.18 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 1 | 0.18 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 3 | 0.18 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 8 | 0.18 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 12 | 0.18 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 12 | 0.18 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 12 | 0.18 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 12 | 0.18 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 12 | 0.18 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 12 | 0.18 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 15 | 0.18 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 15 | 0.18 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 15 | 0.18 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 15 | 0.18 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 15 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 15 | 0.18 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 2 | 0.18 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 3 | 0.18 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 13 | 0.18 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 14 | 0.18 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 14 | 0.18 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD2 | 12 | 0.18 |
| (1,657) | 1:152:A:LYS:H | 1:152:A:LYS:HD3 | 12 | 0.18 |
| (1,630) | 1:98:A:PRO:HA | 1:99:A:GLU:HG2 | 13 | 0.18 |
| (1,630) | 1:98:A:PRO:HA | 1:99:A:GLU:HG3 | 13 | 0.18 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 14 | 0.18 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 14 | 0.18 |
| (1,598) | 1:93:A:GLU:HA | 1:94:A:ALA:HB1 | 15 | 0.18 |
| (1,598) | 1:93:A:GLU:HA | 1:94:A:ALA:HB2 | 15 | 0.18 |
| (1,598) | 1:93:A:GLU:HA | 1:94:A:ALA:HB3 | 15 | 0.18 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD2 | 8 | 0.18 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD3 | 8 | 0.18 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD2 | 13 | 0.18 |
| (1,574) | 1:159:A:ASN:HB3 | 1:161:A:LYS:HD3 | 13 | 0.18 |
| (1,547) | 1:107:A:LEU:HA | 1:107:A:LEU:HG | 4 | 0.18 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 10 | 0.18 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 17 | 0.18 |
| (1,507) | 1:70:A:THR:HG21 | 1:86:A:GLU:HA | 10 | 0.18 |
| (1,507) | 1:70:A:THR:HG22 | 1:86:A:GLU:HA | 10 | 0.18 |
| (1,507) | 1:70:A:THR:HG23 | 1:86:A:GLU:HA | 10 | 0.18 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 3 | 0.18 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 7 | 0.18 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 14 | 0.18 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 18 | 0.18 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 2 | 0.18 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 16 | 0.18 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 16 | 0.18 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 16 | 0.18 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD11 | 8 | 0.18 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD12 | 8 | 0.18 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD13 | 8 | 0.18 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 13 | 0.18 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 8 | 0.18 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 8 | 0.18 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 8 | 0.18 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG11 | 8 | 0.18 |
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG12 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,288) | 1:116:A:GLN:H | 1:143:A:VAL:HG13 | 8 | 0.18 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 14 | 0.18 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 14 | 0.18 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 14 | 0.18 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 15 | 0.18 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 15 | 0.18 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 15 | 0.18 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 16 | 0.18 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 16 | 0.18 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 16 | 0.18 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 16 | 0.18 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 15 | 0.18 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 15 | 0.18 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 15 | 0.18 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 9 | 0.18 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 9 | 0.18 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 9 | 0.18 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 3 | 0.18 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 3 | 0.18 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 3 | 0.18 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 5 | 0.18 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 5 | 0.18 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 5 | 0.18 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 13 | 0.18 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 12 | 0.18 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 12 | 0.18 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 2 | 0.18 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 2 | 0.18 |
| (1,17) | 1:47:A:THR:HG21 | 1:48:A:ASN:H | 20 | 0.18 |
| (1,17) | 1:47:A:THR:HG22 | 1:48:A:ASN:H | 20 | 0.18 |
| (1,17) | 1:47:A:THR:HG23 | 1:48:A:ASN:H | 20 | 0.18 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 18 | 0.18 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 18 | 0.18 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 18 | 0.18 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 8 | 0.17 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 13 | 0.17 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 13 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 5 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 5 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 5 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 5 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 5 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 5 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 7 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 7 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 7 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 7 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 7 | 0.17 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 7 | 0.17 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 8 | 0.17 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 8 | 0.17 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 8 | 0.17 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 8 | 0.17 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 8 | 0.17 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 8 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 6 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 6 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 6 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 6 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 6 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 6 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 13 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 13 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 13 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 13 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 13 | 0.17 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 13 | 0.17 |
| (1,3903) | 1:177:A:GLU:HB3 | 1:209:A:LEU:HD11 | 1 | 0.17 |
| (1,3903) | 1:177:A:GLU:HB3 | 1:209:A:LEU:HD12 | 1 | 0.17 |
| (1,3903) | 1:177:A:GLU:HB3 | 1:209:A:LEU:HD13 | 1 | 0.17 |
| (1,3903) | 1:177:A:GLU:HB3 | 1:209:A:LEU:HD21 | 1 | 0.17 |
| (1,3903) | 1:177:A:GLU:HB3 | 1:209:A:LEU:HD22 | 1 | 0.17 |
| (1,3903) | 1:177:A:GLU:HB3 | 1:209:A:LEU:HD23 | 1 | 0.17 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 3 | 0.17 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 3 | 0.17 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 3 | 0.17 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 3 | 0.17 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 3 | 0.17 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 20 | 0.17 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 20 | 0.17 |
| (1,3830) | 1:126:A:ALA:HA | 1:133:A:TRP:HB2 | 8 | 0.17 |
| (1,3830) | 1:126:A:ALA:HA | 1:133:A:TRP:HB3 | 8 | 0.17 |
| (1,3740) | 1:110:A:VAL:HG11 | 1:123:A:LYS:H | 6 | 0.17 |
| (1,3740) | 1:110:A:VAL:HG12 | 1:123:A:LYS:H | 6 | 0.17 |
| (1,3740) | 1:110:A:VAL:HG13 | 1:123:A:LYS:H | 6 | 0.17 |
| (1,3740) | 1:110:A:VAL:HG21 | 1:123:A:LYS:H | 6 | 0.17 |
| (1,3740) | 1:110:A:VAL:HG22 | 1:123:A:LYS:H | 6 | 0.17 |
| (1,3740) | 1:110:A:VAL:HG23 | 1:123:A:LYS:H | 6 | 0.17 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 8 | 0.17 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 8 | 0.17 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE21 | 14 | 0.17 |
| (1,3591) | 1:75:A:ILE:H | 1:83:A:GLN:HE22 | 14 | 0.17 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 10 | 0.17 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 10 | 0.17 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 19 | 0.17 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 19 | 0.17 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 19 | 0.17 |
| (1,3521) | 1:59:A:ALA:HB1 | 2:12:B:ASN:HB2 | 2 | 0.17 |
| (1,3521) | 1:59:A:ALA:HB2 | 2:12:B:ASN:HB2 | 2 | 0.17 |
| (1,3521) | 1:59:A:ALA:HB3 | 2:12:B:ASN:HB2 | 2 | 0.17 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 1 | 0.17 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 1 | 0.17 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 1 | 0.17 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD11 | 3 | 0.17 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD12 | 3 | 0.17 |
| (1,3517) | 1:51:A:PRO:HG3 | 2:9:B:ILE:HD13 | 3 | 0.17 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 1 | 0.17 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 1 | 0.17 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 1 | 0.17 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 1 | 0.17 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 1 | 0.17 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 1 | 0.17 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 9 | 0.17 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 9 | 0.17 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 9 | 0.17 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG21 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG22 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3478) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG23 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG21 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG22 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG23 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG21 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG22 | 1 | 0.17 |
| (1,3478) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG23 | 1 | 0.17 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 7 | 0.17 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 7 | 0.17 |
| (1,3462) | 2:17:B:LYS:HA | 2:17:B:LYS:HG2 | 10 | 0.17 |
| (1,3411) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB2 | 3 | 0.17 |
| (1,3411) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB2 | 3 | 0.17 |
| (1,3411) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB2 | 3 | 0.17 |
| (1,3400) | 2:5:B:PRO:HA | 2:6:B:VAL:HG11 | 1 | 0.17 |
| (1,3400) | 2:5:B:PRO:HA | 2:6:B:VAL:HG12 | 1 | 0.17 |
| (1,3400) | 2:5:B:PRO:HA | 2:6:B:VAL:HG13 | 1 | 0.17 |
| (1,3352) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HG2 | 14 | 0.17 |
| (1,3352) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HG2 | 14 | 0.17 |
| (1,3277) | 1:69:A:PHE:HD1 | 1:87:A:VAL:HB | 11 | 0.17 |
| (1,3277) | 1:69:A:PHE:HD2 | 1:87:A:VAL:HB | 11 | 0.17 |
| (1,3220) | 1:125:A:TRP:HD1 | 1:126:A:ALA:H | 16 | 0.17 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 11 | 0.17 |
| (1,3160) | 1:133:A:TRP:HH2 | 1:135:A:PHE:HD1 | 7 | 0.17 |
| (1,3160) | 1:133:A:TRP:HH2 | 1:135:A:PHE:HD2 | 7 | 0.17 |
| (1,3155) | 1:56:A:ALA:HB1 | 1:69:A:PHE:HD1 | 19 | 0.17 |
| (1,3155) | 1:56:A:ALA:HB1 | 1:69:A:PHE:HD2 | 19 | 0.17 |
| (1,3155) | 1:56:A:ALA:HB2 | 1:69:A:PHE:HD1 | 19 | 0.17 |
| (1,3155) | 1:56:A:ALA:HB2 | 1:69:A:PHE:HD2 | 19 | 0.17 |
| (1,3155) | 1:56:A:ALA:HB3 | 1:69:A:PHE:HD1 | 19 | 0.17 |
| (1,3155) | 1:56:A:ALA:HB3 | 1:69:A:PHE:HD2 | 19 | 0.17 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 4 | 0.17 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 4 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 16 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 16 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 16 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 16 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 16 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 16 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 19 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 19 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 19 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 19 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 19 | 0.17 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 19 | 0.17 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 11 | 0.17 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 13 | 0.17 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 18 | 0.17 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 14 | 0.17 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 4 | 0.17 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 14 | 0.17 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 14 | 0.17 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 17 | 0.17 |
| (1,3023) | 1:191:A:THR:H | 1:219:A:THR:H | 1 | 0.17 |
| (1,2929) | 1:192:A:ILE:HB | 1:221:A:THR:H | 20 | 0.17 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 5 | 0.17 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 12 | 0.17 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 14 | 0.17 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 20 | 0.17 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 2 | 0.17 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 17 | 0.17 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 16 | 0.17 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 16 | 0.17 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 16 | 0.17 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 17 | 0.17 |
| (1,2754) | 1:153:A:VAL:HB | 1:166:A:ASP:H | 7 | 0.17 |
| (1,2754) | 1:153:A:VAL:HB | 1:166:A:ASP:H | 13 | 0.17 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 18 | 0.17 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 18 | 0.17 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 18 | 0.17 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 18 | 0.17 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 18 | 0.17 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 18 | 0.17 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 13 | 0.17 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 3 | 0.17 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 11 | 0.17 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 13 | 0.17 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 15 | 0.17 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 17 | 0.17 |
| (1,2645) | 1:148:A:SER:H | 1:179:A:LEU:HB3 | 3 | 0.17 |
| (1,2643) | 1:147:A:GLY:HA3 | 1:148:A:SER:H | 19 | 0.17 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 9 | 0.17 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 12 | 0.17 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 17 | 0.17 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 15 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 6 | 0.17 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 1 | 0.17 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 10 | 0.17 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 13 | 0.17 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 16 | 0.17 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 17 | 0.17 |
| (1,2618) | 1:117:A:VAL:HG21 | 1:143:A:VAL:H | 13 | 0.17 |
| (1,2618) | 1:117:A:VAL:HG22 | 1:143:A:VAL:H | 13 | 0.17 |
| (1,2618) | 1:117:A:VAL:HG23 | 1:143:A:VAL:H | 13 | 0.17 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 6 | 0.17 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 6 | 0.17 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 6 | 0.17 |
| (1,2544) | 1:128:A:LEU:HD11 | 1:131:A:LYS:H | 2 | 0.17 |
| (1,2544) | 1:128:A:LEU:HD12 | 1:131:A:LYS:H | 2 | 0.17 |
| (1,2544) | 1:128:A:LEU:HD13 | 1:131:A:LYS:H | 2 | 0.17 |
| (1,2544) | 1:128:A:LEU:HD21 | 1:131:A:LYS:H | 2 | 0.17 |
| (1,2544) | 1:128:A:LEU:HD22 | 1:131:A:LYS:H | 2 | 0.17 |
| (1,2544) | 1:128:A:LEU:HD23 | 1:131:A:LYS:H | 2 | 0.17 |
| (1,2506) | 1:147:A:GLY:HA2 | 1:179:A:LEU:H | 18 | 0.17 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 16 | 0.17 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 16 | 0.17 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 5 | 0.17 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 13 | 0.17 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 10 | 0.17 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 7 | 0.17 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 15 | 0.17 |
| (1,2344) | 1:86:A:GLU:HG2 | 1:87:A:VAL:H | 20 | 0.17 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 11 | 0.17 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 17 | 0.17 |
| (1,2184) | 1:56:A:ALA:H | 1:73:A:VAL:HG11 | 7 | 0.17 |
| (1,2184) | 1:56:A:ALA:H | 1:73:A:VAL:HG12 | 7 | 0.17 |
| (1,2184) | 1:56:A:ALA:H | 1:73:A:VAL:HG13 | 7 | 0.17 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 19 | 0.17 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 19 | 0.17 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 19 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 12 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 12 | 0.17 |
| (1,2101) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 12 | 0.17 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 14 | 0.17 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 14 | 0.17 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 14 | 0.17 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 20 | 0.17 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 20 | 0.17 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 20 | 0.17 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE2 | 2 | 0.17 |
| (1,2044) | 1:198:A:THR:HG21 | 1:225:A:LYS:HE3 | 2 | 0.17 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE2 | 2 | 0.17 |
| (1,2044) | 1:198:A:THR:HG22 | 1:225:A:LYS:HE3 | 2 | 0.17 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE2 | 2 | 0.17 |
| (1,2044) | 1:198:A:THR:HG23 | 1:225:A:LYS:HE3 | 2 | 0.17 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 7 | 0.17 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 4 | 0.17 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 5 | 0.17 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 5 | 0.17 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 11 | 0.17 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 16 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 9 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 9 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 13 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 13 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 14 | 0.17 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 14 | 0.17 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 5 | 0.17 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 18 | 0.17 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 9 | 0.17 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 9 | 0.17 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 9 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 19 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 19 | 0.17 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 19 | 0.17 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 17 | 0.17 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 1 | 0.17 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 1 | 0.17 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 1 | 0.17 |
| (1,1787) | 1:201:A:ILE:HA | 1:205:A:LYS:HG2 | 10 | 0.17 |
| (1,1769) | 1:200:A:ALA:HA | 1:201:A:ILE:HB | 3 | 0.17 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 17 | 0.17 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD11 | 10 | 0.17 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD12 | 10 | 0.17 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD13 | 10 | 0.17 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 4 | 0.17 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 4 | 0.17 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 4 | 0.17 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 12 | 0.17 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 12 | 0.17 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 12 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 8 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 8 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 8 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 15 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 15 | 0.17 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 15 | 0.17 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 1 | 0.17 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 11 | 0.17 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 2 | 0.17 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 7 | 0.17 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 18 | 0.17 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 18 | 0.17 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 18 | 0.17 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 17 | 0.17 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 17 | 0.17 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 17 | 0.17 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 3 | 0.17 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 3 | 0.17 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1549) | 1:184:A:ILE:HD11 | 1:219:A:THR:H | 12 | 0.17 |
| (1,1549) | 1:184:A:ILE:HD12 | 1:219:A:THR:H | 12 | 0.17 |
| (1,1549) | 1:184:A:ILE:HD13 | 1:219:A:THR:H | 12 | 0.17 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 10 | 0.17 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 10 | 0.17 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 10 | 0.17 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 1 | 0.17 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 1 | 0.17 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 20 | 0.17 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 20 | 0.17 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 20 | 0.17 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 18 | 0.17 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 18 | 0.17 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 18 | 0.17 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 20 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 17 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 17 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 17 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 17 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 17 | 0.17 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 17 | 0.17 |
| (1,1470) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HG | 15 | 0.17 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 5 | 0.17 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 5 | 0.17 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 5 | 0.17 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 6 | 0.17 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 14 | 0.17 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 14 | 0.17 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 14 | 0.17 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 18 | 0.17 |
| (1,1387) | 1:172:A:SER:HB3 | 1:174:A:GLU:HB3 | 2 | 0.17 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 18 | 0.17 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 18 | 0.17 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 18 | 0.17 |
| (1,1375) | 1:149:A:ALA:HB1 | 1:170:A:PHE:HA | 13 | 0.17 |
| (1,1375) | 1:149:A:ALA:HB2 | 1:170:A:PHE:HA | 13 | 0.17 |
| (1,1375) | 1:149:A:ALA:HB3 | 1:170:A:PHE:HA | 13 | 0.17 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 8 | 0.17 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 8 | 0.17 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 3 | 0.17 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 7 | 0.17 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 10 | 0.17 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 10 | 0.17 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 10 | 0.17 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 3 | 0.17 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 3 | 0.17 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 3 | 0.17 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG21 | 13 | 0.17 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG22 | 13 | 0.17 |
| (1,1208) | 1:152:A:LYS:HG3 | 1:153:A:VAL:HG23 | 13 | 0.17 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 2 | 0.17 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 20 | 0.17 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 20 | 0.17 |
| (1,1146) | 1:142:A:THR:HA | 1:147:A:GLY:HA3 | 15 | 0.17 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 12 | 0.17 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 12 | 0.17 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 12 | 0.17 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 7 | 0.17 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 7 | 0.17 |
| (1,1097) | 1:140:A:ILE:HG21 | 1:151:A:ALA:H | 2 | 0.17 |
| (1,1097) | 1:140:A:ILE:HG22 | 1:151:A:ALA:H | 2 | 0.17 |
| (1,1097) | 1:140:A:ILE:HG23 | 1:151:A:ALA:H | 2 | 0.17 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 2 | 0.17 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 2 | 0.17 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 2 | 0.17 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 12 | 0.17 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 12 | 0.17 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 12 | 0.17 |
| (1,1050) | 1:139:A:SER:HB3 | 1:150:A:SER:HA | 19 | 0.17 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 8 | 0.17 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 13 | 0.17 |
| (1,990) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HB | 15 | 0.17 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 14 | 0.17 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 14 | 0.17 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 14 | 0.17 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 14 | 0.17 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 14 | 0.17 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 14 | 0.17 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 14 | 0.17 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 13 | 0.17 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 13 | 0.17 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 15 | 0.17 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 15 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 15 | 0.17 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 18 | 0.17 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 18 | 0.17 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 18 | 0.17 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 15 | 0.17 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 15 | 0.17 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 15 | 0.17 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 8 | 0.17 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 15 | 0.17 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 20 | 0.17 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 4 | 0.17 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 18 | 0.17 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 8 | 0.17 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 20 | 0.17 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB2 | 16 | 0.17 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB3 | 16 | 0.17 |
| (1,692) | 1:87:A:VAL:HB | 1:106:A:ALA:HA | 19 | 0.17 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 12 | 0.17 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 8 | 0.17 |
| (1,643) | 1:101:A:VAL:HA | 1:129:A:ASN:HD21 | 18 | 0.17 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 7 | 0.17 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 7 | 0.17 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 7 | 0.17 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 3 | 0.17 |
| (1,609) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 19 | 0.17 |
| (1,609) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 19 | 0.17 |
| (1,609) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 19 | 0.17 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 11 | 0.17 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 11 | 0.17 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 11 | 0.17 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 11 | 0.17 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 11 | 0.17 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 11 | 0.17 |
| (1,535) | 1:99:A:GLU:HB3 | 1:100:A:PRO:HD3 | 15 | 0.17 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 3 | 0.17 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 6 | 0.17 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 16 | 0.17 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 17 | 0.17 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 8 | 0.17 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 7 | 0.17 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 20 | 0.17 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 20 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 10 | 0.17 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 10 | 0.17 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 10 | 0.17 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD11 | 3 | 0.17 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD12 | 3 | 0.17 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD13 | 3 | 0.17 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 5 | 0.17 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 5 | 0.17 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 5 | 0.17 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 5 | 0.17 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 5 | 0.17 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 5 | 0.17 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 19 | 0.17 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 19 | 0.17 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 19 | 0.17 |
| (1,353) | 1:73:A:VAL:HG11 | 1:74:A:ASP:HA | 10 | 0.17 |
| (1,353) | 1:73:A:VAL:HG12 | 1:74:A:ASP:HA | 10 | 0.17 |
| (1,353) | 1:73:A:VAL:HG13 | 1:74:A:ASP:HA | 10 | 0.17 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 14 | 0.17 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 17 | 0.17 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 17 | 0.17 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 17 | 0.17 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 17 | 0.17 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 17 | 0.17 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 17 | 0.17 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB1 | 2 | 0.17 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB2 | 2 | 0.17 |
| (1,264) | 1:63:A:TYR:HB2 | 1:67:A:ALA:HB3 | 2 | 0.17 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 9 | 0.17 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 9 | 0.17 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 9 | 0.17 |
| (1,226) | 1:129:A:ASN:HB3 | 1:130:A:THR:HA | 4 | 0.17 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 14 | 0.17 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 14 | 0.17 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 14 | 0.17 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 15 | 0.17 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 15 | 0.17 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 15 | 0.17 |
| (1,191) | 1:152:A:LYS:H | 1:168:A:ALA:HA | 9 | 0.17 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 11 | 0.17 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 17 | 0.17 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 4 | 0.17 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 4 | 0.17 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 19 | 0.17 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 19 | 0.17 |
| (1,142) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HB3 | 15 | 0.17 |
| (1,142) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HB3 | 15 | 0.17 |
| (1,142) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HB3 | 15 | 0.17 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 6 | 0.17 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 6 | 0.17 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 6 | 0.17 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 16 | 0.17 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 16 | 0.17 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 16 | 0.17 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 19 | 0.17 |
| (1,83) | 1:53:A:THR:HB | 1:76:A:MET:HB3 | 4 | 0.17 |
| (1,63) | 1:52:A:VAL:HG11 | 2:8:B:ILE:HA | 8 | 0.17 |
| (1,63) | 1:52:A:VAL:HG12 | 2:8:B:ILE:HA | 8 | 0.17 |
| (1,63) | 1:52:A:VAL:HG13 | 2:8:B:ILE:HA | 8 | 0.17 |
| (1,56) | 1:51:A:PRO:HB2 | 1:52:A:VAL:HA | 2 | 0.17 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 8 | 0.17 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 18 | 0.17 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 18 | 0.17 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 18 | 0.17 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 17 | 0.17 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 17 | 0.17 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 17 | 0.17 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG2 | 2 | 0.16 |
| (1,4039) | 2:15:B:THR:HG21 | 2:17:B:LYS:HG3 | 2 | 0.16 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG2 | 2 | 0.16 |
| (1,4039) | 2:15:B:THR:HG22 | 2:17:B:LYS:HG3 | 2 | 0.16 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG2 | 2 | 0.16 |
| (1,4039) | 2:15:B:THR:HG23 | 2:17:B:LYS:HG3 | 2 | 0.16 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 11 | 0.16 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 11 | 0.16 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 8 | 0.16 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 8 | 0.16 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 8 | 0.16 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 8 | 0.16 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 8 | 0.16 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 15 | 0.16 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 15 | 0.16 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 15 | 0.16 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 15 | 0.16 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 15 | 0.16 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 15 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 11 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 11 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 11 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 11 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 11 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 11 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 12 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 12 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 12 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 12 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 12 | 0.16 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 12 | 0.16 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 10 | 0.16 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 10 | 0.16 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 19 | 0.16 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 19 | 0.16 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 15 | 0.16 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 15 | 0.16 |
| (1,3768) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HG13 | 3 | 0.16 |
| (1,3768) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HG13 | 3 | 0.16 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD2 | 10 | 0.16 |
| (1,3748) | 1:111:A:HIS:HB3 | 1:120:A:LYS:HD3 | 10 | 0.16 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 19 | 0.16 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 19 | 0.16 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 19 | 0.16 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 17 | 0.16 |
| (1,3620) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB3 | 17 | 0.16 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 14 | 0.16 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 14 | 0.16 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 14 | 0.16 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 14 | 0.16 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 18 | 0.16 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 18 | 0.16 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 18 | 0.16 |
| (1,3519) | 1:51:A:PRO:HG2 | 2:9:B:ILE:HG12 | 16 | 0.16 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 3 | 0.16 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 3 | 0.16 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD1 | 11 | 0.16 |
| (1,3500) | 1:54:A:ILE:HB | 2:10:B:TYR:HD2 | 11 | 0.16 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 19 | 0.16 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 19 | 0.16 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 19 | 0.16 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 12 | 0.16 |
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 12 | 0.16 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 12 | 0.16 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 19 | 0.16 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 19 | 0.16 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 19 | 0.16 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 7 | 0.16 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 7 | 0.16 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 7 | 0.16 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 7 | 0.16 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 7 | 0.16 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 7 | 0.16 |
| (1,3428) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 17 | 0.16 |
| (1,3411) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB2 | 5 | 0.16 |
| (1,3411) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB2 | 5 | 0.16 |
| (1,3411) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB2 | 5 | 0.16 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 13 | 0.16 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 13 | 0.16 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 13 | 0.16 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 8 | 0.16 |
| (1,3301) | 2:17:B:LYS:H | 2:17:B:LYS:HG2 | 7 | 0.16 |
| (1,3274) | 1:111:A:HIS:HD2 | 1:113:A:ASP:H | 12 | 0.16 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 2 | 0.16 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 2 | 0.16 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 8 | 0.16 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 8 | 0.16 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 8 | 0.16 |
| (1,3208) | 1:126:A:ALA:HB1 | 1:133:A:TRP:HD1 | 11 | 0.16 |
| (1,3208) | 1:126:A:ALA:HB2 | 1:133:A:TRP:HD1 | 11 | 0.16 |
| (1,3208) | 1:126:A:ALA:HB3 | 1:133:A:TRP:HD1 | 11 | 0.16 |
| (1,3204) | 1:88:A:GLN:HB3 | 1:90:A:HIS:HE1 | 14 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 3 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 3 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 3 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 3 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 3 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 3 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 4 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 4 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 4 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 4 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 4 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 4 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 15 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 15 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 15 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 15 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 15 | 0.16 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 15 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 3 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 3 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 3 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 3 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 3 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 3 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 9 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 9 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 9 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 9 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 9 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 9 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 11 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 11 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 11 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 11 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 11 | 0.16 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 11 | 0.16 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 9 | 0.16 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 9 | 0.16 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 11 | 0.16 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 11 | 0.16 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 13 | 0.16 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 13 | 0.16 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 13 | 0.16 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 13 | 0.16 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 13 | 0.16 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 13 | 0.16 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 11 | 0.16 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 11 | 0.16 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 8 | 0.16 |
| (1,3084) | 1:116:A:GLN:HB3 | 1:116:A:GLN:HE22 | 13 | 0.16 |
| (1,3082) | 1:116:A:GLN:HE21 | 1:187:A:MET:HB3 | 6 | 0.16 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 4 | 0.16 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 6 | 0.16 |
| (1,3012) | 1:216:A:LEU:HB2 | 1:217:A:GLY:H | 15 | 0.16 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 13 | 0.16 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 13 | 0.16 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 13 | 0.16 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE2 | 6 | 0.16 |
| (1,2965) | 1:202:A:THR:H | 1:205:A:LYS:HE3 | 6 | 0.16 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG21 | 8 | 0.16 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG22 | 8 | 0.16 |
| (1,2948) | 1:198:A:THR:H | 1:201:A:ILE:HG23 | 8 | 0.16 |
| (1,2882) | 1:187:A:MET:H | 1:187:A:MET:HG2 | 19 | 0.16 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 5 | 0.16 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 5 | 0.16 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 15 | 0.16 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 15 | 0.16 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 16 | 0.16 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 4 | 0.16 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 4 | 0.16 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 4 | 0.16 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 13 | 0.16 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 19 | 0.16 |
| (1,2788) | 1:172:A:SER:H | 1:175:A:ASN:H | 18 | 0.16 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 14 | 0.16 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 14 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 14 | 0.16 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 2 | 0.16 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 12 | 0.16 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 13 | 0.16 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 17 | 0.16 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 4 | 0.16 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 9 | 0.16 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 4 | 0.16 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 6 | 0.16 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 11 | 0.16 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 11 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 10 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 10 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 10 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 11 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 11 | 0.16 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 11 | 0.16 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 7 | 0.16 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 10 | 0.16 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 13 | 0.16 |
| (1,2537) | 1:129:A:ASN:HB2 | 1:130:A:THR:H | 7 | 0.16 |
| (1,2508) | 1:201:A:ILE:HD11 | 1:205:A:LYS:H | 1 | 0.16 |
| (1,2508) | 1:201:A:ILE:HD12 | 1:205:A:LYS:H | 1 | 0.16 |
| (1,2508) | 1:201:A:ILE:HD13 | 1:205:A:LYS:H | 1 | 0.16 |
| (1,2506) | 1:147:A:GLY:HA2 | 1:179:A:LEU:H | 9 | 0.16 |
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 15 | 0.16 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE1 | 6 | 0.16 |
| (1,2492) | 1:121:A:GLY:H | 1:135:A:PHE:HE2 | 6 | 0.16 |
| (1,2437) | 1:82:A:LEU:HG | 1:113:A:ASP:H | 7 | 0.16 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 15 | 0.16 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG11 | 7 | 0.16 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG12 | 7 | 0.16 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG13 | 7 | 0.16 |
| (1,2378) | 1:94:A:ALA:H | 1:97:A:GLN:H | 13 | 0.16 |
| (1,2374) | 1:221:A:THR:HB | 1:222:A:ILE:H | 11 | 0.16 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 15 | 0.16 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 5 | 0.16 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 11 | 0.16 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 12 | 0.16 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG11 | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG12 | 5 | 0.16 |
| (1,2331) | 1:85:A:ASP:H | 1:110:A:VAL:HG13 | 5 | 0.16 |
| (1,2311) | 1:82:A:LEU:H | 1:112:A:TYR:HD1 | 17 | 0.16 |
| (1,2311) | 1:82:A:LEU:H | 1:112:A:TYR:HD2 | 17 | 0.16 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 20 | 0.16 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 10 | 0.16 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 19 | 0.16 |
| (1,2288) | 1:75:A:ILE:HB | 1:76:A:MET:H | 8 | 0.16 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 3 | 0.16 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 11 | 0.16 |
| (1,2211) | 1:60:A:LYS:H | 1:60:A:LYS:HE3 | 6 | 0.16 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 3 | 0.16 |
| (1,2143) | 1:50:A:LEU:H | 1:51:A:PRO:HD2 | 17 | 0.16 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 6 | 0.16 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 6 | 0.16 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG21 | 3 | 0.16 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG22 | 3 | 0.16 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG23 | 3 | 0.16 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 2 | 0.16 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 2 | 0.16 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 2 | 0.16 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 18 | 0.16 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 18 | 0.16 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 18 | 0.16 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 18 | 0.16 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 18 | 0.16 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 18 | 0.16 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 4 | 0.16 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 4 | 0.16 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 4 | 0.16 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 4 | 0.16 |
| (1,1897) | 1:202:A:THR:HG21 | 1:204:A:GLU:HA | 10 | 0.16 |
| (1,1897) | 1:202:A:THR:HG22 | 1:204:A:GLU:HA | 10 | 0.16 |
| (1,1897) | 1:202:A:THR:HG23 | 1:204:A:GLU:HA | 10 | 0.16 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 19 | 0.16 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB1 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB2 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB3 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB1 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB2 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB3 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB1 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB2 | 14 | 0.16 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB3 | 14 | 0.16 |
| (1,1795) | 1:201:A:ILE:HD11 | 1:202:A:THR:H | 5 | 0.16 |
| (1,1795) | 1:201:A:ILE:HD12 | 1:202:A:THR:H | 5 | 0.16 |
| (1,1795) | 1:201:A:ILE:HD13 | 1:202:A:THR:H | 5 | 0.16 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 8 | 0.16 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 16 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG21 | 1:196:A:ASN:HA | 12 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG22 | 1:196:A:ASN:HA | 12 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG23 | 1:196:A:ASN:HA | 12 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG21 | 1:196:A:ASN:HA | 14 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG22 | 1:196:A:ASN:HA | 14 | 0.16 |
| (1,1707) | 1:194:A:ILE:HG23 | 1:196:A:ASN:HA | 14 | 0.16 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 19 | 0.16 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 19 | 0.16 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 19 | 0.16 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 4 | 0.16 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 4 | 0.16 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 4 | 0.16 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 10 | 0.16 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 10 | 0.16 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 10 | 0.16 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 9 | 0.16 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 4 | 0.16 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 6 | 0.16 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD2 | 3 | 0.16 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD3 | 3 | 0.16 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 4 | 0.16 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 4 | 0.16 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 4 | 0.16 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 13 | 0.16 |
| (1,1542) | 1:184:A:ILE:HA | 1:189:A:VAL:HB | 7 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 4 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 4 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 7 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 7 | 0.16 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 7 | 0.16 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 11 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 13 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 13 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 13 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 17 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 17 | 0.16 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 17 | 0.16 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 15 | 0.16 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 15 | 0.16 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 15 | 0.16 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 5 | 0.16 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB1 | 12 | 0.16 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB2 | 12 | 0.16 |
| (1,1460) | 1:146:A:PRO:HG3 | 1:178:A:ALA:HB3 | 12 | 0.16 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 16 | 0.16 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 20 | 0.16 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 11 | 0.16 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 11 | 0.16 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 11 | 0.16 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 6 | 0.16 |
| (1,1360) | 1:153:A:VAL:HB | 1:166:A:ASP:HB2 | 17 | 0.16 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 2 | 0.16 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 2 | 0.16 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 10 | 0.16 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 10 | 0.16 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 12 | 0.16 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 13 | 0.16 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 13 | 0.16 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 13 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD11 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD12 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD13 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD21 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD22 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD23 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD11 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD12 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD13 | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD21 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD22 | 9 | 0.16 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD23 | 9 | 0.16 |
| (1,1146) | 1:142:A:THR:HA | 1:147:A:GLY:HA3 | 3 | 0.16 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 1 | 0.16 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 1 | 0.16 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 1 | 0.16 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 1 | 0.16 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 1 | 0.16 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 1 | 0.16 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 17 | 0.16 |
| (1,1099) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HB3 | 18 | 0.16 |
| (1,1099) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HB3 | 18 | 0.16 |
| (1,1099) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HB3 | 18 | 0.16 |
| (1,1085) | 1:140:A:ILE:HD11 | 1:149:A:ALA:H | 9 | 0.16 |
| (1,1085) | 1:140:A:ILE:HD12 | 1:149:A:ALA:H | 9 | 0.16 |
| (1,1085) | 1:140:A:ILE:HD13 | 1:149:A:ALA:H | 9 | 0.16 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 3 | 0.16 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 3 | 0.16 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 3 | 0.16 |
| (1,1082) | 1:140:A:ILE:HD11 | 1:142:A:THR:H | 16 | 0.16 |
| (1,1082) | 1:140:A:ILE:HD12 | 1:142:A:THR:H | 16 | 0.16 |
| (1,1082) | 1:140:A:ILE:HD13 | 1:142:A:THR:H | 16 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 1 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 1 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 1 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 1 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 1 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 1 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 2 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 2 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 2 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 2 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 2 | 0.16 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 2 | 0.16 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB1 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB2 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD11 | 1:67:A:ALA:HB3 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB1 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB2 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD12 | 1:67:A:ALA:HB3 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB1 | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB2 | 15 | 0.16 |
| (1,926) | 1:54:A:ILE:HD13 | 1:67:A:ALA:HB3 | 15 | 0.16 |
| (1,893) | 1:155:A:LYS:HE3 | 1:166:A:ASP:H | 17 | 0.16 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 10 | 0.16 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 15 | 0.16 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 2 | 0.16 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 2 | 0.16 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 2 | 0.16 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 6 | 0.16 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 6 | 0.16 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 6 | 0.16 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE2 | 6 | 0.16 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE3 | 6 | 0.16 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE2 | 15 | 0.16 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE3 | 15 | 0.16 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 16 | 0.16 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 16 | 0.16 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 16 | 0.16 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 16 | 0.16 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 16 | 0.16 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 16 | 0.16 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 6 | 0.16 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 16 | 0.16 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 14 | 0.16 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 9 | 0.16 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB2 | 3 | 0.16 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB3 | 3 | 0.16 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 3 | 0.16 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 13 | 0.16 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 20 | 0.16 |
| (1,632) | 1:51:A:PRO:HA | 2:6:B:VAL:HG21 | 12 | 0.16 |
| (1,632) | 1:51:A:PRO:HA | 2:6:B:VAL:HG22 | 12 | 0.16 |
| (1,632) | 1:51:A:PRO:HA | 2:6:B:VAL:HG23 | 12 | 0.16 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 11 | 0.16 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 11 | 0.16 |
| (1,572) | 1:92:A:LYS:HD2 | 1:93:A:GLU:H | 15 | 0.16 |
| (1,572) | 1:92:A:LYS:HD3 | 1:93:A:GLU:H | 15 | 0.16 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 19 | 0.16 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 5 | 0.16 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 12 | 0.16 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 10 | 0.16 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 16 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 16 | 0.16 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 14 | 0.16 |
| (1,460) | 1:81:A:ARG:HB3 | 1:81:A:ARG:HD3 | 4 | 0.16 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 13 | 0.16 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 13 | 0.16 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 13 | 0.16 |
| (1,409) | 1:75:A:ILE:HG21 | 1:76:A:MET:HA | 17 | 0.16 |
| (1,409) | 1:75:A:ILE:HG22 | 1:76:A:MET:HA | 17 | 0.16 |
| (1,409) | 1:75:A:ILE:HG23 | 1:76:A:MET:HA | 17 | 0.16 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 12 | 0.16 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 12 | 0.16 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 12 | 0.16 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 14 | 0.16 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 14 | 0.16 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 14 | 0.16 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 17 | 0.16 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 13 | 0.16 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 13 | 0.16 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 13 | 0.16 |
| (1,261) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HZ | 4 | 0.16 |
| (1,261) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HZ | 4 | 0.16 |
| (1,261) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HZ | 4 | 0.16 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 1 | 0.16 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 1 | 0.16 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 1 | 0.16 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 2 | 0.16 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 2 | 0.16 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 2 | 0.16 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 6 | 0.16 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 6 | 0.16 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 6 | 0.16 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 16 | 0.16 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 16 | 0.16 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 16 | 0.16 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG21 | 13 | 0.16 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG22 | 13 | 0.16 |
| (1,178) | 1:58:A:HIS:HB2 | 1:70:A:THR:HG23 | 13 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 5 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 5 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 5 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 8 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 8 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 17 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 17 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 17 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 20 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 20 | 0.16 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 20 | 0.16 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD11 | 16 | 0.16 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD12 | 16 | 0.16 |
| (1,122) | 1:53:A:THR:H | 1:54:A:ILE:HD13 | 16 | 0.16 |
| (1,92) | 1:53:A:THR:HG21 | 2:9:B:ILE:HG12 | 12 | 0.16 |
| (1,92) | 1:53:A:THR:HG22 | 2:9:B:ILE:HG12 | 12 | 0.16 |
| (1,92) | 1:53:A:THR:HG23 | 2:9:B:ILE:HG12 | 12 | 0.16 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 12 | 0.16 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 17 | 0.16 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 17 | 0.16 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 17 | 0.16 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 6 | 0.16 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 6 | 0.16 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 6 | 0.16 |
| (1,33) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB3 | 14 | 0.16 |
| (1,33) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB3 | 14 | 0.16 |
| (1,33) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB3 | 14 | 0.16 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 5 | 0.15 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 5 | 0.15 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 4 | 0.15 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 4 | 0.15 |
| (1,4014) | 2:10:B:TYR:HD1 | 2:19:B:GLN:HE21 | 18 | 0.15 |
| (1,4014) | 2:10:B:TYR:HD1 | 2:19:B:GLN:HE22 | 18 | 0.15 |
| (1,4014) | 2:10:B:TYR:HD2 | 2:19:B:GLN:HE21 | 18 | 0.15 |
| (1,4014) | 2:10:B:TYR:HD2 | 2:19:B:GLN:HE22 | 18 | 0.15 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 16 | 0.15 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 16 | 0.15 |
| (1,3990) | 1:220:A:LEU:HD11 | 1:221:A:THR:H | 2 | 0.15 |
| (1,3990) | 1:220:A:LEU:HD12 | 1:221:A:THR:H | 2 | 0.15 |
| (1,3990) | 1:220:A:LEU:HD13 | 1:221:A:THR:H | 2 | 0.15 |
| (1,3990) | 1:220:A:LEU:HD21 | 1:221:A:THR:H | 2 | 0.15 |
| (1,3990) | 1:220:A:LEU:HD22 | 1:221:A:THR:H | 2 | 0.15 |
| (1,3990) | 1:220:A:LEU:HD23 | 1:221:A:THR:H | 2 | 0.15 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 1 | 0.15 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 1 | 0.15 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 1 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 1 | 0.15 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 1 | 0.15 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 1 | 0.15 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG2 | 15 | 0.15 |
| (1,3956) | 1:202:A:THR:HG21 | 1:204:A:GLU:HG3 | 15 | 0.15 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG2 | 15 | 0.15 |
| (1,3956) | 1:202:A:THR:HG22 | 1:204:A:GLU:HG3 | 15 | 0.15 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG2 | 15 | 0.15 |
| (1,3956) | 1:202:A:THR:HG23 | 1:204:A:GLU:HG3 | 15 | 0.15 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD21 | 16 | 0.15 |
| (1,3951) | 1:194:A:ILE:HA | 1:195:A:ASN:HD22 | 16 | 0.15 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 10 | 0.15 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 10 | 0.15 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 10 | 0.15 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 10 | 0.15 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 10 | 0.15 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 10 | 0.15 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 7 | 0.15 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 7 | 0.15 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 7 | 0.15 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 7 | 0.15 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 7 | 0.15 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 7 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD11 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD12 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD13 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD21 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD22 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HD23 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD11 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD12 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD13 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD21 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD22 | 17 | 0.15 |
| (1,3905) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HD23 | 17 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD11 | 4 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD12 | 4 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD13 | 4 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD21 | 4 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD22 | 4 | 0.15 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD23 | 4 | 0.15 |
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB2 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3884) | 1:169:A:THR:HG21 | 1:171:A:ASP:HB3 | 8 | 0.15 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB2 | 8 | 0.15 |
| (1,3884) | 1:169:A:THR:HG22 | 1:171:A:ASP:HB3 | 8 | 0.15 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB2 | 8 | 0.15 |
| (1,3884) | 1:169:A:THR:HG23 | 1:171:A:ASP:HB3 | 8 | 0.15 |
| (1,3865) | 1:151:A:ALA:HA | 1:167:A:ASP:HB2 | 10 | 0.15 |
| (1,3865) | 1:151:A:ALA:HA | 1:167:A:ASP:HB3 | 10 | 0.15 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 18 | 0.15 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 18 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 11 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 11 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 11 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 11 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 11 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 11 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 19 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 19 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 19 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 19 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 19 | 0.15 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 19 | 0.15 |
| (1,3714) | 1:105:A:ASP:HB2 | 1:107:A:LEU:HG | 15 | 0.15 |
| (1,3714) | 1:105:A:ASP:HB3 | 1:107:A:LEU:HG | 15 | 0.15 |
| (1,3672) | 1:91:A:GLN:HB2 | 1:92:A:LYS:H | 20 | 0.15 |
| (1,3672) | 1:91:A:GLN:HB3 | 1:92:A:LYS:H | 20 | 0.15 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 15 | 0.15 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 15 | 0.15 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 15 | 0.15 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 15 | 0.15 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 10 | 0.15 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 10 | 0.15 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 9 | 0.15 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 9 | 0.15 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB2 | 14 | 0.15 |
| (1,3550) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 14 | 0.15 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB2 | 14 | 0.15 |
| (1,3550) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 14 | 0.15 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB2 | 14 | 0.15 |
| (1,3550) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 14 | 0.15 |
| (1,3538) | 1:48:A:ASN:HD21 | 1:49:A:ASP:H | 3 | 0.15 |
| (1,3538) | 1:48:A:ASN:HD22 | 1:49:A:ASP:H | 3 | 0.15 |
| (1,3521) | 1:59:A:ALA:HB1 | 2:12:B:ASN:HB2 | 12 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3521) | 1:59:A:ALA:HB2 | 2:12:B:ASN:HB2 | 12 | 0.15 |
| (1,3521) | 1:59:A:ALA:HB3 | 2:12:B:ASN:HB2 | 12 | 0.15 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 16 | 0.15 |
| (1,3488) | 1:54:A:ILE:HD11 | 2:11:B:CYS:H | 3 | 0.15 |
| (1,3488) | 1:54:A:ILE:HD12 | 2:11:B:CYS:H | 3 | 0.15 |
| (1,3488) | 1:54:A:ILE:HD13 | 2:11:B:CYS:H | 3 | 0.15 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 1 | 0.15 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 1 | 0.15 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 1 | 0.15 |
| (1,3479) | 1:53:A:THR:HG21 | 2:9:B:ILE:HB | 14 | 0.15 |
| (1,3479) | 1:53:A:THR:HG22 | 2:9:B:ILE:HB | 14 | 0.15 |
| (1,3479) | 1:53:A:THR:HG23 | 2:9:B:ILE:HB | 14 | 0.15 |
| (1,3462) | 2:17:B:LYS:HA | 2:17:B:LYS:HG2 | 5 | 0.15 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 14 | 0.15 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 14 | 0.15 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 14 | 0.15 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 14 | 0.15 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 14 | 0.15 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 14 | 0.15 |
| (1,3396) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HA | 9 | 0.15 |
| (1,3396) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HA | 9 | 0.15 |
| (1,3396) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HA | 9 | 0.15 |
| (1,3373) | 2:19:B:GLN:HB2 | 2:21:B:MET:H | 4 | 0.15 |
| (1,3373) | 2:19:B:GLN:HB3 | 2:21:B:MET:H | 4 | 0.15 |
| (1,3321) | 2:9:B:ILE:H | 2:9:B:ILE:HG12 | 5 | 0.15 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 13 | 0.15 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 13 | 0.15 |
| (1,3264) | 1:58:A:HIS:HD2 | 1:60:A:LYS:H | 6 | 0.15 |
| (1,3229) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD21 | 18 | 0.15 |
| (1,3204) | 1:88:A:GLN:HB3 | 1:90:A:HIS:HE1 | 16 | 0.15 |
| (1,3176) | 1:170:A:PHE:HD1 | 1:172:A:SER:H | 12 | 0.15 |
| (1,3176) | 1:170:A:PHE:HD2 | 1:172:A:SER:H | 12 | 0.15 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 17 | 0.15 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 17 | 0.15 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 17 | 0.15 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 17 | 0.15 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 17 | 0.15 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 17 | 0.15 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB1 | 15 | 0.15 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB2 | 15 | 0.15 |
| (1,3165) | 1:135:A:PHE:HD1 | 1:138:A:ALA:HB3 | 15 | 0.15 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB1 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB2 | 15 | 0.15 |
| (1,3165) | 1:135:A:PHE:HD2 | 1:138:A:ALA:HB3 | 15 | 0.15 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 1 | 0.15 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 1 | 0.15 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 8 | 0.15 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 8 | 0.15 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 15 | 0.15 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 15 | 0.15 |
| (1,3119) | 1:63:A:TYR:HE1 | 2:21:B:MET:HA | 3 | 0.15 |
| (1,3119) | 1:63:A:TYR:HE2 | 2:21:B:MET:HA | 3 | 0.15 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 2 | 0.15 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 2 | 0.15 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 2 | 0.15 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 1 | 0.15 |
| (1,3092) | 1:49:A:ASP:H | 1:50:A:LEU:HG | 20 | 0.15 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 15 | 0.15 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 15 | 0.15 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 15 | 0.15 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 1 | 0.15 |
| (1,3085) | 1:68:A:VAL:HA | 1:88:A:GLN:HE22 | 7 | 0.15 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 4 | 0.15 |
| (1,3083) | 1:116:A:GLN:HE21 | 1:187:A:MET:HG3 | 12 | 0.15 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 5 | 0.15 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 10 | 0.15 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 14 | 0.15 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 14 | 0.15 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 14 | 0.15 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 3 | 0.15 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 10 | 0.15 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 15 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 1 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 1 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 3 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 3 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 9 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 9 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 18 | 0.15 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 18 | 0.15 |
| (1,2854) | 1:180:A:ILE:HG13 | 1:182:A:HIS:H | 9 | 0.15 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 13 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 3 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 3 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 3 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 13 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 13 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 13 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 20 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 20 | 0.15 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 20 | 0.15 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 3 | 0.15 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 15 | 0.15 |
| (1,2758) | 1:153:A:VAL:HG11 | 1:166:A:ASP:H | 1 | 0.15 |
| (1,2758) | 1:153:A:VAL:HG12 | 1:166:A:ASP:H | 1 | 0.15 |
| (1,2758) | 1:153:A:VAL:HG13 | 1:166:A:ASP:H | 1 | 0.15 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 7 | 0.15 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 13 | 0.15 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 13 | 0.15 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 13 | 0.15 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 13 | 0.15 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 13 | 0.15 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 13 | 0.15 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 10 | 0.15 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 18 | 0.15 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 8 | 0.15 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 12 | 0.15 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 12 | 0.15 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 12 | 0.15 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 6 | 0.15 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 8 | 0.15 |
| (1,2635) | 1:146:A:PRO:HB2 | 1:147:A:GLY:H | 14 | 0.15 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 16 | 0.15 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 15 | 0.15 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 15 | 0.15 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 15 | 0.15 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 18 | 0.15 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 18 | 0.15 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 18 | 0.15 |
| (1,2605) | 1:142:A:THR:H | 1:148:A:SER:HA | 12 | 0.15 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 2 | 0.15 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 4 | 0.15 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 11 | 0.15 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 11 | 0.15 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 11 | 0.15 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 12 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 12 | 0.15 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 12 | 0.15 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 12 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD11 | 12 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD12 | 12 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD13 | 12 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD11 | 18 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD12 | 18 | 0.15 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD13 | 18 | 0.15 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 18 | 0.15 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 11 | 0.15 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 18 | 0.15 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 1 | 0.15 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 20 | 0.15 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 4 | 0.15 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 4 | 0.15 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 20 | 0.15 |
| (1,2260) | 1:57:A:ASP:HB3 | 1:72:A:SER:H | 16 | 0.15 |
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 10 | 0.15 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 4 | 0.15 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 7 | 0.15 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 18 | 0.15 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 18 | 0.15 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 18 | 0.15 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG21 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG22 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG21 | 1:73:A:VAL:HG23 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG21 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG22 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG22 | 1:73:A:VAL:HG23 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG21 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG22 | 20 | 0.15 |
| (1,2100) | 1:70:A:THR:HG23 | 1:73:A:VAL:HG23 | 20 | 0.15 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG21 | 10 | 0.15 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG22 | 10 | 0.15 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG23 | 10 | 0.15 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 7 | 0.15 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 7 | 0.15 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 7 | 0.15 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 5 | 0.15 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 5 | 0.15 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 17 | 0.15 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 17 | 0.15 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 17 | 0.15 |
| (1,2001) | 1:185:A:LYS:HA | 1:216:A:LEU:HG | 19 | 0.15 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 3 | 0.15 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 3 | 0.15 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 3 | 0.15 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 3 | 0.15 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 3 | 0.15 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 3 | 0.15 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 1 | 0.15 |
| (1,1912) | 1:209:A:LEU:HB3 | 1:211:A:ALA:H | 13 | 0.15 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 1 | 0.15 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 1 | 0.15 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 18 | 0.15 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 18 | 0.15 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB1 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB2 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB3 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB1 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB2 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB3 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB1 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB2 | 19 | 0.15 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB3 | 19 | 0.15 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 7 | 0.15 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 7 | 0.15 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 7 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 18 | 0.15 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 18 | 0.15 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 7 | 0.15 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 13 | 0.15 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 13 | 0.15 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 13 | 0.15 |
| (1,1738) | 1:197:A:ALA:HA | 1:222:A:ILE:HG12 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 6 | 0.15 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 8 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB1 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB2 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB3 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB1 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB2 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB3 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB1 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB2 | 1 | 0.15 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB3 | 1 | 0.15 |
| (1,1656) | 1:192:A:ILE:HD11 | 1:220:A:LEU:H | 4 | 0.15 |
| (1,1656) | 1:192:A:ILE:HD12 | 1:220:A:LEU:H | 4 | 0.15 |
| (1,1656) | 1:192:A:ILE:HD13 | 1:220:A:LEU:H | 4 | 0.15 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 20 | 0.15 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 20 | 0.15 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 20 | 0.15 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 6 | 0.15 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 6 | 0.15 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 6 | 0.15 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD2 | 10 | 0.15 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD3 | 10 | 0.15 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD2 | 14 | 0.15 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD3 | 14 | 0.15 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG21 | 17 | 0.15 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG22 | 17 | 0.15 |
| (1,1603) | 1:117:A:VAL:H | 1:186:A:THR:HG23 | 17 | 0.15 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 14 | 0.15 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 14 | 0.15 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 14 | 0.15 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 1 | 0.15 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 16 | 0.15 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 19 | 0.15 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 20 | 0.15 |
| (1,1552) | 1:184:A:ILE:HD11 | 1:191:A:THR:HA | 2 | 0.15 |
| (1,1552) | 1:184:A:ILE:HD12 | 1:191:A:THR:HA | 2 | 0.15 |
| (1,1552) | 1:184:A:ILE:HD13 | 1:191:A:THR:HA | 2 | 0.15 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 5 | 0.15 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 5 | 0.15 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 5 | 0.15 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 16 | 0.15 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 16 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 16 | 0.15 |
| (1,1535) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG12 | 16 | 0.15 |
| (1,1535) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG12 | 16 | 0.15 |
| (1,1535) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG12 | 16 | 0.15 |
| (1,1519) | 1:142:A:THR:HG21 | 1:182:A:HIS:HA | 12 | 0.15 |
| (1,1519) | 1:142:A:THR:HG22 | 1:182:A:HIS:HA | 12 | 0.15 |
| (1,1519) | 1:142:A:THR:HG23 | 1:182:A:HIS:HA | 12 | 0.15 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 8 | 0.15 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 12 | 0.15 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 13 | 0.15 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 11 | 0.15 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 11 | 0.15 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 11 | 0.15 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 1 | 0.15 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 1 | 0.15 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 1 | 0.15 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 9 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD11 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD12 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD13 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD11 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD12 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD13 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD11 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD12 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD13 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD11 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD12 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD13 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD11 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD12 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD13 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD11 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD12 | 7 | 0.15 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD13 | 7 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD11 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD12 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD13 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD21 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD22 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD23 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD11 | 12 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD12 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD13 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD21 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD22 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD23 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD11 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD12 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD13 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD21 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD22 | 12 | 0.15 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD23 | 12 | 0.15 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 6 | 0.15 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 7 | 0.15 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 11 | 0.15 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 3 | 0.15 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 7 | 0.15 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 14 | 0.15 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 15 | 0.15 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 15 | 0.15 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 15 | 0.15 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 17 | 0.15 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 17 | 0.15 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 17 | 0.15 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 7 | 0.15 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 7 | 0.15 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 13 | 0.15 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 13 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 4 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 14 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 20 | 0.15 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 20 | 0.15 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 12 | 0.15 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 12 | 0.15 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 16 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 18 | 0.15 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 18 | 0.15 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 20 | 0.15 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 20 | 0.15 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 20 | 0.15 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG21 | 5 | 0.15 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG22 | 5 | 0.15 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG23 | 5 | 0.15 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG21 | 1 | 0.15 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG22 | 1 | 0.15 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG23 | 1 | 0.15 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 4 | 0.15 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 20 | 0.15 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 6 | 0.15 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 19 | 0.15 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 1 | 0.15 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 1 | 0.15 |
| (1,1157) | 1:140:A:ILE:HG21 | 1:148:A:SER:HB2 | 19 | 0.15 |
| (1,1157) | 1:140:A:ILE:HG21 | 1:148:A:SER:HB3 | 19 | 0.15 |
| (1,1157) | 1:140:A:ILE:HG22 | 1:148:A:SER:HB2 | 19 | 0.15 |
| (1,1157) | 1:140:A:ILE:HG22 | 1:148:A:SER:HB3 | 19 | 0.15 |
| (1,1157) | 1:140:A:ILE:HG23 | 1:148:A:SER:HB2 | 19 | 0.15 |
| (1,1157) | 1:140:A:ILE:HG23 | 1:148:A:SER:HB3 | 19 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 8 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 8 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 8 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 17 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 17 | 0.15 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 17 | 0.15 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG2 | 5 | 0.15 |
| (1,1107) | 1:118:A:ILE:HD11 | 1:141:A:GLU:HG3 | 5 | 0.15 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG2 | 5 | 0.15 |
| (1,1107) | 1:118:A:ILE:HD12 | 1:141:A:GLU:HG3 | 5 | 0.15 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG2 | 5 | 0.15 |
| (1,1107) | 1:118:A:ILE:HD13 | 1:141:A:GLU:HG3 | 5 | 0.15 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 5 | 0.15 |
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 5 | 0.15 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 5 | 0.15 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 6 | 0.15 |
| (1,1006) | 1:136:A:TYR:HB3 | 1:152:A:LYS:HA | 19 | 0.15 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 2 | 0.15 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,985) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG21 | 19 | 0.15 |
| (1,985) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG22 | 19 | 0.15 |
| (1,985) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG23 | 19 | 0.15 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG11 | 19 | 0.15 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG12 | 19 | 0.15 |
| (1,978) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HG13 | 19 | 0.15 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG11 | 20 | 0.15 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG12 | 20 | 0.15 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG13 | 20 | 0.15 |
| (1,943) | 1:128:A:LEU:HD11 | 1:129:A:ASN:HB2 | 13 | 0.15 |
| (1,943) | 1:128:A:LEU:HD12 | 1:129:A:ASN:HB2 | 13 | 0.15 |
| (1,943) | 1:128:A:LEU:HD13 | 1:129:A:ASN:HB2 | 13 | 0.15 |
| (1,943) | 1:128:A:LEU:HD21 | 1:129:A:ASN:HB2 | 13 | 0.15 |
| (1,943) | 1:128:A:LEU:HD22 | 1:129:A:ASN:HB2 | 13 | 0.15 |
| (1,943) | 1:128:A:LEU:HD23 | 1:129:A:ASN:HB2 | 13 | 0.15 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 18 | 0.15 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 18 | 0.15 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 6 | 0.15 |
| (1,880) | 1:173:A:TYR:HA | 1:201:A:ILE:HB | 5 | 0.15 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 16 | 0.15 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 16 | 0.15 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 16 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE2 | 8 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE3 | 8 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE2 | 14 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE3 | 14 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE2 | 18 | 0.15 |
| (1,869) | 1:120:A:LYS:HG2 | 1:120:A:LYS:HE3 | 18 | 0.15 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 5 | 0.15 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 5 | 0.15 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 5 | 0.15 |
| (1,845) | 1:117:A:VAL:HG21 | 1:118:A:ILE:HG12 | 12 | 0.15 |
| (1,845) | 1:117:A:VAL:HG22 | 1:118:A:ILE:HG12 | 12 | 0.15 |
| (1,845) | 1:117:A:VAL:HG23 | 1:118:A:ILE:HG12 | 12 | 0.15 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 5 | 0.15 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 5 | 0.15 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 5 | 0.15 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 5 | 0.15 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 5 | 0.15 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 5 | 0.15 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG2 | 18 | 0.15 |
| (1,839) | 1:118:A:ILE:HG21 | 1:141:A:GLU:HG3 | 18 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG2 | 18 | 0.15 |
| (1,839) | 1:118:A:ILE:HG22 | 1:141:A:GLU:HG3 | 18 | 0.15 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG2 | 18 | 0.15 |
| (1,839) | 1:118:A:ILE:HG23 | 1:141:A:GLU:HG3 | 18 | 0.15 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 9 | 0.15 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 9 | 0.15 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 9 | 0.15 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 11 | 0.15 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 11 | 0.15 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 11 | 0.15 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 16 | 0.15 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 16 | 0.15 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 16 | 0.15 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 4 | 0.15 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 9 | 0.15 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 10 | 0.15 |
| (1,776) | 1:113:A:ASP:HA | 1:118:A:ILE:HG12 | 2 | 0.15 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 13 | 0.15 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 1 | 0.15 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 16 | 0.15 |
| (1,717) | 1:107:A:LEU:HG | 1:108:A:GLY:H | 18 | 0.15 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 17 | 0.15 |
| (1,685) | 1:104:A:VAL:HB | 1:126:A:ALA:H | 20 | 0.15 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 12 | 0.15 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 16 | 0.15 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 20 | 0.15 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 20 | 0.15 |
| (1,620) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD2 | 8 | 0.15 |
| (1,609) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB2 | 15 | 0.15 |
| (1,609) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB2 | 15 | 0.15 |
| (1,609) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB2 | 15 | 0.15 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 6 | 0.15 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 6 | 0.15 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 7 | 0.15 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 7 | 0.15 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 9 | 0.15 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 9 | 0.15 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 16 | 0.15 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 16 | 0.15 |
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG2 | 1 | 0.15 |
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG3 | 1 | 0.15 |
| (1,594) | 1:93:A:GLU:HA | 1:93:A:GLU:HG2 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 1 | 0.15 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 1 | 0.15 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 1 | 0.15 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 1 | 0.15 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 1 | 0.15 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 1 | 0.15 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 4 | 0.15 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 4 | 0.15 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 4 | 0.15 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 4 | 0.15 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 4 | 0.15 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 4 | 0.15 |
| (1,524) | 1:86:A:GLU:H | 1:87:A:VAL:HA | 20 | 0.15 |
| (1,513) | 1:123:A:LYS:HB3 | 1:123:A:LYS:HD3 | 4 | 0.15 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 14 | 0.15 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 14 | 0.15 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 14 | 0.15 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 3 | 0.15 |
| (1,410) | 1:53:A:THR:H | 1:75:A:ILE:HG21 | 13 | 0.15 |
| (1,410) | 1:53:A:THR:H | 1:75:A:ILE:HG22 | 13 | 0.15 |
| (1,410) | 1:53:A:THR:H | 1:75:A:ILE:HG23 | 13 | 0.15 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD11 | 20 | 0.15 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD12 | 20 | 0.15 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD13 | 20 | 0.15 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD11 | 14 | 0.15 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD12 | 14 | 0.15 |
| (1,379) | 1:54:A:ILE:HA | 1:75:A:ILE:HD13 | 14 | 0.15 |
| (1,357) | 1:73:A:VAL:HG11 | 1:87:A:VAL:H | 14 | 0.15 |
| (1,357) | 1:73:A:VAL:HG12 | 1:87:A:VAL:H | 14 | 0.15 |
| (1,357) | 1:73:A:VAL:HG13 | 1:87:A:VAL:H | 14 | 0.15 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 10 | 0.15 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 10 | 0.15 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 10 | 0.15 |
| (1,320) | 1:58:A:HIS:HB3 | 1:71:A:GLY:HA3 | 13 | 0.15 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 19 | 0.15 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 19 | 0.15 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 19 | 0.15 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 19 | 0.15 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 19 | 0.15 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 19 | 0.15 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 8 | 0.15 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 8 | 0.15 |
| (1,251) | 1:222:A:ILE:HD11 | 1:224:A:LEU:HA | 5 | 0.15 |
| (1,251) | 1:222:A:ILE:HD12 | 1:224:A:LEU:HA | 5 | 0.15 |
| (1,251) | 1:222:A:ILE:HD13 | 1:224:A:LEU:HA | 5 | 0.15 |
| (1,245) | 1:63:A:TYR:HA | 1:64:A:PRO:HG2 | 12 | 0.15 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 9 | 0.15 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 9 | 0.15 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 9 | 0.15 |
| (1,191) | 1:152:A:LYS:H | 1:168:A:ALA:HA | 17 | 0.15 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 1 | 0.15 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 6 | 0.15 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 6 | 0.15 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 6 | 0.15 |
| (1,179) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB2 | 7 | 0.15 |
| (1,179) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB2 | 7 | 0.15 |
| (1,179) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB2 | 7 | 0.15 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 3 | 0.15 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 3 | 0.15 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 8 | 0.15 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 8 | 0.15 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 9 | 0.15 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 9 | 0.15 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 9 | 0.15 |
| (1,121) | 1:54:A:ILE:HD11 | 1:75:A:ILE:HG13 | 16 | 0.15 |
| (1,121) | 1:54:A:ILE:HD12 | 1:75:A:ILE:HG13 | 16 | 0.15 |
| (1,121) | 1:54:A:ILE:HD13 | 1:75:A:ILE:HG13 | 16 | 0.15 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 5 | 0.15 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 5 | 0.15 |
| (1,80) | 1:53:A:THR:HA | 2:9:B:ILE:HA | 3 | 0.15 |
| (1,79) | 1:70:A:THR:HA | 1:86:A:GLU:HB3 | 9 | 0.15 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG21 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG22 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HG23 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG21 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG22 | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,67) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HG23 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG21 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG22 | 11 | 0.15 |
| (1,67) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HG23 | 11 | 0.15 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 2 | 0.15 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 14 | 0.15 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 3 | 0.15 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 3 | 0.15 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 3 | 0.15 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 12 | 0.15 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 10 | 0.15 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 10 | 0.15 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 10 | 0.15 |
| (1,17) | 1:47:A:THR:HG21 | 1:48:A:ASN:H | 18 | 0.15 |
| (1,17) | 1:47:A:THR:HG22 | 1:48:A:ASN:H | 18 | 0.15 |
| (1,17) | 1:47:A:THR:HG23 | 1:48:A:ASN:H | 18 | 0.15 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 14 | 0.15 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 14 | 0.15 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 14 | 0.15 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 6 | 0.14 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 6 | 0.14 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB2 | 15 | 0.14 |
| (1,4018) | 2:12:B:ASN:HA | 2:13:B:ARG:HB3 | 15 | 0.14 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 1 | 0.14 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 1 | 0.14 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 1 | 0.14 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 1 | 0.14 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 1 | 0.14 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 1 | 0.14 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 1 | 0.14 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 1 | 0.14 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 10 | 0.14 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 10 | 0.14 |
| (1,3654) | 1:88:A:GLN:HG2 | 1:90:A:HIS:HE1 | 5 | 0.14 |
| (1,3654) | 1:88:A:GLN:HG3 | 1:90:A:HIS:HE1 | 5 | 0.14 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 4 | 0.14 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 4 | 0.14 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 4 | 0.14 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 4 | 0.14 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG11 | 20 | 0.14 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG12 | 20 | 0.14 |
| (1,3544) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HG13 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG11 | 20 | 0.14 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG12 | 20 | 0.14 |
| (1,3544) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HG13 | 20 | 0.14 |
| (1,3523) | 1:52:A:VAL:HG11 | 2:9:B:ILE:H | 5 | 0.14 |
| (1,3523) | 1:52:A:VAL:HG12 | 2:9:B:ILE:H | 5 | 0.14 |
| (1,3523) | 1:52:A:VAL:HG13 | 2:9:B:ILE:H | 5 | 0.14 |
| (1,3522) | 1:56:A:ALA:HB1 | 2:12:B:ASN:HA | 12 | 0.14 |
| (1,3522) | 1:56:A:ALA:HB2 | 2:12:B:ASN:HA | 12 | 0.14 |
| (1,3522) | 1:56:A:ALA:HB3 | 2:12:B:ASN:HA | 12 | 0.14 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 20 | 0.14 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 8 | 0.14 |
| (1,3493) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HA | 1 | 0.14 |
| (1,3493) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HA | 1 | 0.14 |
| (1,3493) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HA | 1 | 0.14 |
| (1,3492) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB2 | 15 | 0.14 |
| (1,3492) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB2 | 15 | 0.14 |
| (1,3492) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB2 | 15 | 0.14 |
| (1,3462) | 2:17:B:LYS:HA | 2:17:B:LYS:HG2 | 4 | 0.14 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 1 | 0.14 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 1 | 0.14 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 1 | 0.14 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 1 | 0.14 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 1 | 0.14 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 1 | 0.14 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD1 | 6 | 0.14 |
| (1,3439) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HD2 | 6 | 0.14 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD1 | 6 | 0.14 |
| (1,3439) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HD2 | 6 | 0.14 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD1 | 6 | 0.14 |
| (1,3439) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HD2 | 6 | 0.14 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB2 | 16 | 0.14 |
| (1,3348) | 2:10:B:TYR:HE1 | 2:19:B:GLN:HB3 | 16 | 0.14 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB2 | 16 | 0.14 |
| (1,3348) | 2:10:B:TYR:HE2 | 2:19:B:GLN:HB3 | 16 | 0.14 |
| (1,3276) | 1:111:A:HIS:HE1 | 1:120:A:LYS:HG2 | 19 | 0.14 |
| (1,3274) | 1:111:A:HIS:HD2 | 1:113:A:ASP:H | 10 | 0.14 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD2 | 20 | 0.14 |
| (1,3266) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HD3 | 20 | 0.14 |
| (1,3229) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD21 | 17 | 0.14 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG21 | 13 | 0.14 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG22 | 13 | 0.14 |
| (1,3217) | 1:133:A:TRP:HZ2 | 1:154:A:ILE:HG23 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3155) | 1:56:A:ALA:HB1 | 1:69:A:PHE:HD1 | 6 | 0.14 |
| (1,3155) | 1:56:A:ALA:HB1 | 1:69:A:PHE:HD2 | 6 | 0.14 |
| (1,3155) | 1:56:A:ALA:HB2 | 1:69:A:PHE:HD1 | 6 | 0.14 |
| (1,3155) | 1:56:A:ALA:HB2 | 1:69:A:PHE:HD2 | 6 | 0.14 |
| (1,3155) | 1:56:A:ALA:HB3 | 1:69:A:PHE:HD1 | 6 | 0.14 |
| (1,3155) | 1:56:A:ALA:HB3 | 1:69:A:PHE:HD2 | 6 | 0.14 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 16 | 0.14 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 16 | 0.14 |
| (1,3147) | 1:173:A:TYR:HA | 1:173:A:TYR:HD1 | 19 | 0.14 |
| (1,3147) | 1:173:A:TYR:HA | 1:173:A:TYR:HD2 | 19 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 3 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 3 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 3 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 3 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 3 | 0.14 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 3 | 0.14 |
| (1,3126) | 1:112:A:TYR:HE1 | 1:114:A:ASP:H | 18 | 0.14 |
| (1,3126) | 1:112:A:TYR:HE2 | 1:114:A:ASP:H | 18 | 0.14 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 16 | 0.14 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 16 | 0.14 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 16 | 0.14 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD11 | 20 | 0.14 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD12 | 20 | 0.14 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD13 | 20 | 0.14 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 1 | 0.14 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 10 | 0.14 |
| (1,3063) | 1:125:A:TRP:HH2 | 1:127:A:ASN:HD22 | 13 | 0.14 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 19 | 0.14 |
| (1,3012) | 1:216:A:LEU:HB2 | 1:217:A:GLY:H | 12 | 0.14 |
| (1,3003) | 1:180:A:ILE:HD11 | 1:212:A:LYS:H | 12 | 0.14 |
| (1,3003) | 1:180:A:ILE:HD12 | 1:212:A:LYS:H | 12 | 0.14 |
| (1,3003) | 1:180:A:ILE:HD13 | 1:212:A:LYS:H | 12 | 0.14 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 11 | 0.14 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 11 | 0.14 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 11 | 0.14 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 18 | 0.14 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 18 | 0.14 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 18 | 0.14 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD11 | 12 | 0.14 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD12 | 12 | 0.14 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD13 | 12 | 0.14 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 18 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2874) | 1:186:A:THR:H | 1:187:A:MET:HB2 | 5 | 0.14 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 12 | 0.14 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 12 | 0.14 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 16 | 0.14 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 16 | 0.14 |
| (1,2849) | 1:181:A:GLU:H | 1:182:A:HIS:HB3 | 5 | 0.14 |
| (1,2829) | 1:177:A:GLU:H | 1:178:A:ALA:HA | 7 | 0.14 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 4 | 0.14 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 6 | 0.14 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 6 | 0.14 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 6 | 0.14 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 6 | 0.14 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 8 | 0.14 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 8 | 0.14 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 8 | 0.14 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 2 | 0.14 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 5 | 0.14 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 20 | 0.14 |
| (1,2792) | 1:172:A:SER:H | 1:175:A:ASN:HB3 | 11 | 0.14 |
| (1,2773) | 1:170:A:PHE:H | 1:198:A:THR:H | 16 | 0.14 |
| (1,2722) | 1:157:A:LEU:HB2 | 1:158:A:ASP:H | 8 | 0.14 |
| (1,2701) | 1:133:A:TRP:HH2 | 1:155:A:LYS:H | 13 | 0.14 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 4 | 0.14 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 14 | 0.14 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 19 | 0.14 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 13 | 0.14 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 13 | 0.14 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 13 | 0.14 |
| (1,2605) | 1:142:A:THR:H | 1:148:A:SER:HA | 2 | 0.14 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 1 | 0.14 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 17 | 0.14 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 17 | 0.14 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 17 | 0.14 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 1 | 0.14 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 11 | 0.14 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG11 | 11 | 0.14 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG12 | 11 | 0.14 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG13 | 11 | 0.14 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 20 | 0.14 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD1 | 9 | 0.14 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD2 | 9 | 0.14 |
| (1,2303) | 1:77:A:GLN:HB2 | 1:80:A:SER:H | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2294) | 1:76:A:MET:HB3 | 1:77:A:GLN:H | 13 | 0.14 |
| (1,2294) | 1:76:A:MET:HB3 | 1:77:A:GLN:H | 15 | 0.14 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 6 | 0.14 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 13 | 0.14 |
| (1,2288) | 1:75:A:ILE:HB | 1:76:A:MET:H | 15 | 0.14 |
| (1,2279) | 1:75:A:ILE:H | 1:84:A:ALA:H | 6 | 0.14 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 9 | 0.14 |
| (1,2252) | 1:71:A:GLY:H | 1:86:A:GLU:HG2 | 10 | 0.14 |
| (1,2251) | 1:71:A:GLY:H | 1:86:A:GLU:HB3 | 11 | 0.14 |
| (1,2219) | 1:81:A:ARG:H | 1:115:A:ASN:H | 9 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 2 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 4 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 5 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 11 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 14 | 0.14 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 15 | 0.14 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 3 | 0.14 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 11 | 0.14 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 4 | 0.14 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD11 | 6 | 0.14 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD12 | 6 | 0.14 |
| (1,2140) | 1:49:A:ASP:H | 1:50:A:LEU:HD13 | 6 | 0.14 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE1 | 9 | 0.14 |
| (1,2126) | 1:80:A:SER:HB3 | 1:112:A:TYR:HE2 | 9 | 0.14 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 9 | 0.14 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 9 | 0.14 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 9 | 0.14 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 5 | 0.14 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 5 | 0.14 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 5 | 0.14 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 19 | 0.14 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 19 | 0.14 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 19 | 0.14 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD21 | 10 | 0.14 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD22 | 10 | 0.14 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD23 | 10 | 0.14 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD21 | 19 | 0.14 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD22 | 19 | 0.14 |
| (1,2093) | 1:50:A:LEU:HA | 1:50:A:LEU:HD23 | 19 | 0.14 |
| (1,2088) | 1:196:A:ASN:HA | 1:225:A:LYS:HB3 | 18 | 0.14 |
| (1,2026) | 1:47:A:THR:HG21 | 1:50:A:LEU:HG | 12 | 0.14 |
| (1,2026) | 1:47:A:THR:HG22 | 1:50:A:LEU:HG | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2026) | 1:47:A:THR:HG23 | 1:50:A:LEU:HG | 12 | 0.14 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 12 | 0.14 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 12 | 0.14 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 12 | 0.14 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 3 | 0.14 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 3 | 0.14 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 7 | 0.14 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 7 | 0.14 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 15 | 0.14 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 15 | 0.14 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB1 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB2 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB3 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB1 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB2 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB3 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB1 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB2 | 2 | 0.14 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB3 | 2 | 0.14 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 17 | 0.14 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 17 | 0.14 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 17 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 13 | 0.14 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 13 | 0.14 |
| (1,1815) | 1:201:A:ILE:HG21 | 1:205:A:LYS:H | 9 | 0.14 |
| (1,1815) | 1:201:A:ILE:HG22 | 1:205:A:LYS:H | 9 | 0.14 |
| (1,1815) | 1:201:A:ILE:HG23 | 1:205:A:LYS:H | 9 | 0.14 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 16 | 0.14 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 16 | 0.14 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 16 | 0.14 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 5 | 0.14 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 5 | 0.14 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 5 | 0.14 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 14 | 0.14 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 17 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1713) | 1:194:A:ILE:HG21 | 1:195:A:ASN:HA | 3 | 0.14 |
| (1,1713) | 1:194:A:ILE:HG22 | 1:195:A:ASN:HA | 3 | 0.14 |
| (1,1713) | 1:194:A:ILE:HG23 | 1:195:A:ASN:HA | 3 | 0.14 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD11 | 11 | 0.14 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD12 | 11 | 0.14 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD13 | 11 | 0.14 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD11 | 12 | 0.14 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD12 | 12 | 0.14 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD13 | 12 | 0.14 |
| (1,1658) | 1:163:A:LEU:H | 1:192:A:ILE:HG12 | 18 | 0.14 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD11 | 7 | 0.14 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD12 | 7 | 0.14 |
| (1,1650) | 1:191:A:THR:HB | 1:192:A:ILE:HD13 | 7 | 0.14 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 5 | 0.14 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 2 | 0.14 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 2 | 0.14 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 2 | 0.14 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 5 | 0.14 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 5 | 0.14 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 5 | 0.14 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 17 | 0.14 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 17 | 0.14 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 17 | 0.14 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 5 | 0.14 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 14 | 0.14 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 17 | 0.14 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 4 | 0.14 |
| (1,1570) | 1:184:A:ILE:HG21 | 1:216:A:LEU:HA | 1 | 0.14 |
| (1,1570) | 1:184:A:ILE:HG22 | 1:216:A:LEU:HA | 1 | 0.14 |
| (1,1570) | 1:184:A:ILE:HG23 | 1:216:A:LEU:HA | 1 | 0.14 |
| (1,1567) | 1:184:A:ILE:HG21 | 1:189:A:VAL:H | 3 | 0.14 |
| (1,1567) | 1:184:A:ILE:HG22 | 1:189:A:VAL:H | 3 | 0.14 |
| (1,1567) | 1:184:A:ILE:HG23 | 1:189:A:VAL:H | 3 | 0.14 |
| (1,1545) | 1:184:A:ILE:HA | 1:189:A:VAL:HA | 1 | 0.14 |
| (1,1545) | 1:184:A:ILE:HA | 1:189:A:VAL:HA | 3 | 0.14 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 10 | 0.14 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 10 | 0.14 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 7 | 0.14 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 10 | 0.14 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 17 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 4 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 4 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 9 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 9 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 9 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 18 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 18 | 0.14 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 18 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD11 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD12 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD13 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD21 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD22 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB1 | 1:179:A:LEU:HD23 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD11 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD12 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD13 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD21 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD22 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB2 | 1:179:A:LEU:HD23 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD11 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD12 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD13 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD21 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD22 | 1 | 0.14 |
| (1,1480) | 1:176:A:ALA:HB3 | 1:179:A:LEU:HD23 | 1 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 2 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 2 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 2 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 2 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 2 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 2 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 4 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 4 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 4 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 4 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 4 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 4 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 13 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 13 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 13 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 13 | 0.14 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 13 | 0.14 |
| (1,1475) | 1:141:A:GLU:HA | 1:179:A:LEU:HD11 | 5 | 0.14 |
| (1,1475) | 1:141:A:GLU:HA | 1:179:A:LEU:HD12 | 5 | 0.14 |
| (1,1475) | 1:141:A:GLU:HA | 1:179:A:LEU:HD13 | 5 | 0.14 |
| (1,1475) | 1:141:A:GLU:HA | 1:179:A:LEU:HD21 | 5 | 0.14 |
| (1,1475) | 1:141:A:GLU:HA | 1:179:A:LEU:HD22 | 5 | 0.14 |
| (1,1475) | 1:141:A:GLU:HA | 1:179:A:LEU:HD23 | 5 | 0.14 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 8 | 0.14 |
| (1,1397) | 1:174:A:GLU:HA | 1:177:A:GLU:HA | 7 | 0.14 |
| (1,1381) | 1:225:A:LYS:HB2 | 1:225:A:LYS:HE2 | 2 | 0.14 |
| (1,1381) | 1:225:A:LYS:HB2 | 1:225:A:LYS:HE3 | 2 | 0.14 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE2 | 3 | 0.14 |
| (1,1362) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HE3 | 3 | 0.14 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE2 | 3 | 0.14 |
| (1,1362) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HE3 | 3 | 0.14 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB2 | 6 | 0.14 |
| (1,1347) | 1:155:A:LYS:H | 1:164:A:GLU:HB3 | 6 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 11 | 0.14 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 11 | 0.14 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 14 | 0.14 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 14 | 0.14 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 17 | 0.14 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 17 | 0.14 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 15 | 0.14 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 15 | 0.14 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 15 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 4 | 0.14 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 13 | 0.14 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 2 | 0.14 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG21 | 9 | 0.14 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG22 | 9 | 0.14 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG23 | 9 | 0.14 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 16 | 0.14 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 16 | 0.14 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 16 | 0.14 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD2 | 1 | 0.14 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD3 | 1 | 0.14 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD2 | 16 | 0.14 |
| (1,1211) | 1:153:A:VAL:HB | 1:155:A:LYS:HD3 | 16 | 0.14 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 11 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB1 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB2 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB1 | 1:168:A:ALA:HB3 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB1 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB2 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB2 | 1:168:A:ALA:HB3 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB1 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB2 | 7 | 0.14 |
| (1,1176) | 1:151:A:ALA:HB3 | 1:168:A:ALA:HB3 | 7 | 0.14 |
| (1,1139) | 1:93:A:GLU:H | 1:94:A:ALA:HB1 | 11 | 0.14 |
| (1,1139) | 1:93:A:GLU:H | 1:94:A:ALA:HB2 | 11 | 0.14 |
| (1,1139) | 1:93:A:GLU:H | 1:94:A:ALA:HB3 | 11 | 0.14 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 15 | 0.14 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 15 | 0.14 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 15 | 0.14 |
| (1,1111) | 1:116:A:GLN:HA | 1:142:A:THR:HA | 2 | 0.14 |
| (1,1110) | 1:117:A:VAL:HB | 1:142:A:THR:HA | 2 | 0.14 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG2 | 18 | 0.14 |
| (1,1106) | 1:118:A:ILE:HB | 1:141:A:GLU:HG3 | 18 | 0.14 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 12 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 9 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 9 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 9 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 11 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 11 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 11 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 19 | 0.14 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 19 | 0.14 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 2 | 0.14 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 3 | 0.14 |
| (1,1028) | 1:120:A:LYS:HB2 | 1:138:A:ALA:HA | 15 | 0.14 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD2 | 10 | 0.14 |
| (1,1016) | 1:137:A:ASP:HB2 | 1:152:A:LYS:HD3 | 10 | 0.14 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 18 | 0.14 |
| (1,1002) | 1:123:A:LYS:HD3 | 1:136:A:TYR:HB3 | 5 | 0.14 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 15 | 0.14 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 16 | 0.14 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 10 | 0.14 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 10 | 0.14 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 10 | 0.14 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 12 | 0.14 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 12 | 0.14 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 12 | 0.14 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 20 | 0.14 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 20 | 0.14 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 20 | 0.14 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 19 | 0.14 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 19 | 0.14 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 12 | 0.14 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 10 | 0.14 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 10 | 0.14 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 10 | 0.14 |
| (1,868) | 1:120:A:LYS:HG3 | 1:120:A:LYS:HE2 | 5 | 0.14 |
| (1,868) | 1:120:A:LYS:HG3 | 1:120:A:LYS:HE3 | 5 | 0.14 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 6 | 0.14 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 6 | 0.14 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 6 | 0.14 |
| (1,815) | 1:117:A:VAL:HG11 | 1:118:A:ILE:HG13 | 16 | 0.14 |
| (1,815) | 1:117:A:VAL:HG12 | 1:118:A:ILE:HG13 | 16 | 0.14 |
| (1,815) | 1:117:A:VAL:HG13 | 1:118:A:ILE:HG13 | 16 | 0.14 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 11 | 0.14 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 17 | 0.14 |
| (1,791) | 1:114:A:ASP:H | 1:115:A:ASN:HB2 | 5 | 0.14 |
| (1,791) | 1:114:A:ASP:H | 1:115:A:ASN:HB3 | 5 | 0.14 |
| (1,786) | 1:113:A:ASP:HA | 1:115:A:ASN:HA | 14 | 0.14 |
| (1,698) | 1:106:A:ALA:HB1 | 1:124:A:GLY:HA2 | 9 | 0.14 |
| (1,698) | 1:106:A:ALA:HB2 | 1:124:A:GLY:HA2 | 9 | 0.14 |
| (1,698) | 1:106:A:ALA:HB3 | 1:124:A:GLY:HA2 | 9 | 0.14 |
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,688) | 1:81:A:ARG:HB3 | 1:113:A:ASP:HB2 | 14 | 0.14 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 4 | 0.14 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 6 | 0.14 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 7 | 0.14 |
| (1,676) | 1:103:A:THR:HG21 | 1:128:A:LEU:H | 10 | 0.14 |
| (1,676) | 1:103:A:THR:HG22 | 1:128:A:LEU:H | 10 | 0.14 |
| (1,676) | 1:103:A:THR:HG23 | 1:128:A:LEU:H | 10 | 0.14 |
| (1,644) | 1:101:A:VAL:HA | 1:129:A:ASN:HD22 | 7 | 0.14 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 10 | 0.14 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 17 | 0.14 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 2 | 0.14 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 2 | 0.14 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 4 | 0.14 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 4 | 0.14 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 11 | 0.14 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 11 | 0.14 |
| (1,537) | 1:68:A:VAL:HG11 | 1:88:A:GLN:HG2 | 17 | 0.14 |
| (1,537) | 1:68:A:VAL:HG12 | 1:88:A:GLN:HG2 | 17 | 0.14 |
| (1,537) | 1:68:A:VAL:HG13 | 1:88:A:GLN:HG2 | 17 | 0.14 |
| (1,537) | 1:68:A:VAL:HG21 | 1:88:A:GLN:HG2 | 17 | 0.14 |
| (1,537) | 1:68:A:VAL:HG22 | 1:88:A:GLN:HG2 | 17 | 0.14 |
| (1,537) | 1:68:A:VAL:HG23 | 1:88:A:GLN:HG2 | 17 | 0.14 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 4 | 0.14 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 5 | 0.14 |
| (1,495) | 1:81:A:ARG:HG3 | 1:83:A:GLN:HG3 | 7 | 0.14 |
| (1,484) | 1:82:A:LEU:HG | 1:83:A:GLN:H | 11 | 0.14 |
| (1,448) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 18 | 0.14 |
| (1,436) | 1:75:A:ILE:HG21 | 1:77:A:GLN:HB2 | 16 | 0.14 |
| (1,436) | 1:75:A:ILE:HG22 | 1:77:A:GLN:HB2 | 16 | 0.14 |
| (1,436) | 1:75:A:ILE:HG23 | 1:77:A:GLN:HB2 | 16 | 0.14 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG2 | 13 | 0.14 |
| (1,432) | 1:53:A:THR:H | 1:76:A:MET:HG3 | 13 | 0.14 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 3 | 0.14 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 3 | 0.14 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 3 | 0.14 |
| (1,422) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB2 | 10 | 0.14 |
| (1,422) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB2 | 10 | 0.14 |
| (1,422) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB2 | 10 | 0.14 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD11 | 5 | 0.14 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD12 | 5 | 0.14 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD13 | 5 | 0.14 |
| (1,348) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HB2 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,348) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HB2 | 6 | 0.14 |
| (1,348) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HB2 | 6 | 0.14 |
| (1,328) | 1:197:A:ALA:H | 1:225:A:LYS:HA | 14 | 0.14 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 4 | 0.14 |
| (1,298) | 1:107:A:LEU:HD11 | 1:123:A:LYS:HA | 12 | 0.14 |
| (1,298) | 1:107:A:LEU:HD12 | 1:123:A:LYS:HA | 12 | 0.14 |
| (1,298) | 1:107:A:LEU:HD13 | 1:123:A:LYS:HA | 12 | 0.14 |
| (1,298) | 1:107:A:LEU:HD21 | 1:123:A:LYS:HA | 12 | 0.14 |
| (1,298) | 1:107:A:LEU:HD22 | 1:123:A:LYS:HA | 12 | 0.14 |
| (1,298) | 1:107:A:LEU:HD23 | 1:123:A:LYS:HA | 12 | 0.14 |
| (1,248) | 1:66:A:ASP:HA | 1:89:A:LEU:H | 9 | 0.14 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE1 | 11 | 0.14 |
| (1,247) | 1:69:A:PHE:HB2 | 2:10:B:TYR:HE2 | 11 | 0.14 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE1 | 11 | 0.14 |
| (1,247) | 1:69:A:PHE:HB3 | 2:10:B:TYR:HE2 | 11 | 0.14 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 8 | 0.14 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 8 | 0.14 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 8 | 0.14 |
| (1,165) | 1:56:A:ALA:HB1 | 1:73:A:VAL:HA | 5 | 0.14 |
| (1,165) | 1:56:A:ALA:HB2 | 1:73:A:VAL:HA | 5 | 0.14 |
| (1,165) | 1:56:A:ALA:HB3 | 1:73:A:VAL:HA | 5 | 0.14 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 3 | 0.14 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 3 | 0.14 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 3 | 0.14 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 9 | 0.14 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 9 | 0.14 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 13 | 0.14 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 13 | 0.14 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 16 | 0.14 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 16 | 0.14 |
| (1,143) | 1:53:A:THR:HG21 | 1:55:A:ASN:HB3 | 4 | 0.14 |
| (1,143) | 1:53:A:THR:HG22 | 1:55:A:ASN:HB3 | 4 | 0.14 |
| (1,143) | 1:53:A:THR:HG23 | 1:55:A:ASN:HB3 | 4 | 0.14 |
| (1,143) | 1:53:A:THR:HG21 | 1:55:A:ASN:HB3 | 7 | 0.14 |
| (1,143) | 1:53:A:THR:HG22 | 1:55:A:ASN:HB3 | 7 | 0.14 |
| (1,143) | 1:53:A:THR:HG23 | 1:55:A:ASN:HB3 | 7 | 0.14 |
| (1,133) | 1:54:A:ILE:HG21 | 1:69:A:PHE:HZ | 3 | 0.14 |
| (1,133) | 1:54:A:ILE:HG22 | 1:69:A:PHE:HZ | 3 | 0.14 |
| (1,133) | 1:54:A:ILE:HG23 | 1:69:A:PHE:HZ | 3 | 0.14 |
| (1,115) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB3 | 14 | 0.14 |
| (1,115) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB3 | 14 | 0.14 |
| (1,115) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB3 | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 1 | 0.14 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 1 | 0.14 |
| (1,82) | 1:53:A:THR:HB | 1:54:A:ILE:HG13 | 10 | 0.14 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 9 | 0.14 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 13 | 0.14 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 10 | 0.14 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 19 | 0.14 |
| (1,48) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD3 | 10 | 0.14 |
| (1,48) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD3 | 10 | 0.14 |
| (1,48) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD3 | 10 | 0.14 |
| (1,47) | 1:51:A:PRO:HG2 | 2:8:B:ILE:HA | 19 | 0.14 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 19 | 0.14 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 20 | 0.14 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 19 | 0.14 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 19 | 0.14 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 19 | 0.14 |
| (1,33) | 1:153:A:VAL:HG21 | 1:166:A:ASP:HB3 | 8 | 0.14 |
| (1,33) | 1:153:A:VAL:HG22 | 1:166:A:ASP:HB3 | 8 | 0.14 |
| (1,33) | 1:153:A:VAL:HG23 | 1:166:A:ASP:HB3 | 8 | 0.14 |
| (1,17) | 1:47:A:THR:HG21 | 1:48:A:ASN:H | 9 | 0.14 |
| (1,17) | 1:47:A:THR:HG22 | 1:48:A:ASN:H | 9 | 0.14 |
| (1,17) | 1:47:A:THR:HG23 | 1:48:A:ASN:H | 9 | 0.14 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 19 | 0.14 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 19 | 0.14 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 19 | 0.14 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD2 | 3 | 0.13 |
| (1,4049) | 2:20:B:ARG:HB2 | 2:20:B:ARG:HD3 | 3 | 0.13 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD2 | 3 | 0.13 |
| (1,4049) | 2:20:B:ARG:HB3 | 2:20:B:ARG:HD3 | 3 | 0.13 |
| (1,4036) | 2:14:B:ARG:HG2 | 2:15:B:THR:HA | 16 | 0.13 |
| (1,4036) | 2:14:B:ARG:HG3 | 2:15:B:THR:HA | 16 | 0.13 |
| (1,3950) | 1:193:A:THR:HG21 | 1:195:A:ASN:HD21 | 2 | 0.13 |
| (1,3950) | 1:193:A:THR:HG21 | 1:195:A:ASN:HD22 | 2 | 0.13 |
| (1,3950) | 1:193:A:THR:HG22 | 1:195:A:ASN:HD21 | 2 | 0.13 |
| (1,3950) | 1:193:A:THR:HG22 | 1:195:A:ASN:HD22 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3950) | 1:193:A:THR:HG23 | 1:195:A:ASN:HD21 | 2 | 0.13 |
| (1,3950) | 1:193:A:THR:HG23 | 1:195:A:ASN:HD22 | 2 | 0.13 |
| (1,3946) | 1:190:A:LYS:HE2 | 1:219:A:THR:H | 20 | 0.13 |
| (1,3946) | 1:190:A:LYS:HE3 | 1:219:A:THR:H | 20 | 0.13 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 9 | 0.13 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 9 | 0.13 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 9 | 0.13 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 9 | 0.13 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 9 | 0.13 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 9 | 0.13 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 11 | 0.13 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 11 | 0.13 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 11 | 0.13 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 11 | 0.13 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 11 | 0.13 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 11 | 0.13 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 20 | 0.13 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 20 | 0.13 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 20 | 0.13 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 20 | 0.13 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 20 | 0.13 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 20 | 0.13 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 7 | 0.13 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 7 | 0.13 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 14 | 0.13 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 14 | 0.13 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD11 | 13 | 0.13 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD12 | 13 | 0.13 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD13 | 13 | 0.13 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD21 | 13 | 0.13 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD22 | 13 | 0.13 |
| (1,3902) | 1:177:A:GLU:HB2 | 1:209:A:LEU:HD23 | 13 | 0.13 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD11 | 12 | 0.13 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD12 | 12 | 0.13 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD13 | 12 | 0.13 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD21 | 12 | 0.13 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD22 | 12 | 0.13 |
| (1,3891) | 1:173:A:TYR:HB2 | 1:209:A:LEU:HD23 | 12 | 0.13 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 5 | 0.13 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 5 | 0.13 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB2 | 9 | 0.13 |
| (1,3860) | 1:150:A:SER:H | 1:150:A:SER:HB3 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 10 | 0.13 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 10 | 0.13 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 12 | 0.13 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 12 | 0.13 |
| (1,3838) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA2 | 12 | 0.13 |
| (1,3838) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA2 | 12 | 0.13 |
| (1,3830) | 1:126:A:ALA:HA | 1:133:A:TRP:HB2 | 18 | 0.13 |
| (1,3830) | 1:126:A:ALA:HA | 1:133:A:TRP:HB3 | 18 | 0.13 |
| (1,3773) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 12 | 0.13 |
| (1,3773) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG3 | 12 | 0.13 |
| (1,3773) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 12 | 0.13 |
| (1,3773) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG3 | 12 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG11 | 1:123:A:LYS:H | 20 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG12 | 1:123:A:LYS:H | 20 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG13 | 1:123:A:LYS:H | 20 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG21 | 1:123:A:LYS:H | 20 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG22 | 1:123:A:LYS:H | 20 | 0.13 |
| (1,3740) | 1:110:A:VAL:HG23 | 1:123:A:LYS:H | 20 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 2 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 2 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 2 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 2 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 2 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 2 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 9 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 9 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 9 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 9 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 9 | 0.13 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 9 | 0.13 |
| (1,3707) | 1:102:A:ARG:HG2 | 1:103:A:THR:H | 6 | 0.13 |
| (1,3707) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 6 | 0.13 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 13 | 0.13 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 13 | 0.13 |
| (1,3706) | 1:102:A:ARG:HB2 | 2:8:B:ILE:HG12 | 15 | 0.13 |
| (1,3706) | 1:102:A:ARG:HB3 | 2:8:B:ILE:HG12 | 15 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD11 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD12 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD13 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD21 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD22 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG2 | 1:107:A:LEU:HD23 | 1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD11 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD12 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD13 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD21 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD22 | 1 | 0.13 |
| (1,3655) | 1:88:A:GLN:HG3 | 1:107:A:LEU:HD23 | 1 | 0.13 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 9 | 0.13 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 9 | 0.13 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB2 | 10 | 0.13 |
| (1,3587) | 1:73:A:VAL:HA | 1:74:A:ASP:HB3 | 10 | 0.13 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD11 | 19 | 0.13 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD12 | 19 | 0.13 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD13 | 19 | 0.13 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD21 | 19 | 0.13 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD22 | 19 | 0.13 |
| (1,3582) | 1:68:A:VAL:H | 1:89:A:LEU:HD23 | 19 | 0.13 |
| (1,3543) | 1:49:A:ASP:HB2 | 2:6:B:VAL:HB | 15 | 0.13 |
| (1,3543) | 1:49:A:ASP:HB3 | 2:6:B:VAL:HB | 15 | 0.13 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD11 | 7 | 0.13 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD12 | 7 | 0.13 |
| (1,3513) | 1:54:A:ILE:HB | 2:8:B:ILE:HD13 | 7 | 0.13 |
| (1,3512) | 1:54:A:ILE:HB | 2:10:B:TYR:HB2 | 1 | 0.13 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 6 | 0.13 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 6 | 0.13 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 6 | 0.13 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 3 | 0.13 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 3 | 0.13 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 3 | 0.13 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 3 | 0.13 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 3 | 0.13 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 3 | 0.13 |
| (1,3486) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HA | 3 | 0.13 |
| (1,3486) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HA | 3 | 0.13 |
| (1,3486) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HA | 3 | 0.13 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 16 | 0.13 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 16 | 0.13 |
| (1,3386) | 2:8:B:ILE:HD11 | 2:9:B:ILE:H | 14 | 0.13 |
| (1,3386) | 2:8:B:ILE:HD12 | 2:9:B:ILE:H | 14 | 0.13 |
| (1,3386) | 2:8:B:ILE:HD13 | 2:9:B:ILE:H | 14 | 0.13 |
| (1,3281) | 1:54:A:ILE:HD11 | 1:69:A:PHE:HZ | 17 | 0.13 |
| (1,3281) | 1:54:A:ILE:HD12 | 1:69:A:PHE:HZ | 17 | 0.13 |
| (1,3281) | 1:54:A:ILE:HD13 | 1:69:A:PHE:HZ | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 16 | 0.13 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 16 | 0.13 |
| (1,3255) | 1:116:A:GLN:HA | 1:182:A:HIS:HE1 | 9 | 0.13 |
| (1,3254) | 1:182:A:HIS:HE1 | 1:186:A:THR:HA | 17 | 0.13 |
| (1,3198) | 1:170:A:PHE:HE1 | 1:201:A:ILE:HD11 | 3 | 0.13 |
| (1,3198) | 1:170:A:PHE:HE1 | 1:201:A:ILE:HD12 | 3 | 0.13 |
| (1,3198) | 1:170:A:PHE:HE1 | 1:201:A:ILE:HD13 | 3 | 0.13 |
| (1,3198) | 1:170:A:PHE:HE2 | 1:201:A:ILE:HD11 | 3 | 0.13 |
| (1,3198) | 1:170:A:PHE:HE2 | 1:201:A:ILE:HD12 | 3 | 0.13 |
| (1,3198) | 1:170:A:PHE:HE2 | 1:201:A:ILE:HD13 | 3 | 0.13 |
| (1,3182) | 1:170:A:PHE:HD1 | 1:176:A:ALA:HA | 5 | 0.13 |
| (1,3182) | 1:170:A:PHE:HD2 | 1:176:A:ALA:HA | 5 | 0.13 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 20 | 0.13 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 20 | 0.13 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 20 | 0.13 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 20 | 0.13 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 20 | 0.13 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 20 | 0.13 |
| (1,3156) | 1:125:A:TRP:H | 1:135:A:PHE:HD1 | 6 | 0.13 |
| (1,3156) | 1:125:A:TRP:H | 1:135:A:PHE:HD2 | 6 | 0.13 |
| (1,3150) | 1:173:A:TYR:HE1 | 1:205:A:LYS:HA | 1 | 0.13 |
| (1,3150) | 1:173:A:TYR:HE2 | 1:205:A:LYS:HA | 1 | 0.13 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 9 | 0.13 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 9 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 11 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 11 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 11 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 11 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 11 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 11 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 14 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 14 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 14 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 14 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 14 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 14 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 20 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 20 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 20 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 20 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 20 | 0.13 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 20 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 13 | 0.13 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 13 | 0.13 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD11 | 16 | 0.13 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD12 | 16 | 0.13 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD13 | 16 | 0.13 |
| (1,3091) | 1:83:A:GLN:HB3 | 1:83:A:GLN:HE22 | 9 | 0.13 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 11 | 0.13 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 3 | 0.13 |
| (1,3025) | 1:190:A:LYS:HA | 1:219:A:THR:H | 15 | 0.13 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 2 | 0.13 |
| (1,3014) | 1:184:A:ILE:HG21 | 1:217:A:GLY:H | 13 | 0.13 |
| (1,3014) | 1:184:A:ILE:HG22 | 1:217:A:GLY:H | 13 | 0.13 |
| (1,3014) | 1:184:A:ILE:HG23 | 1:217:A:GLY:H | 13 | 0.13 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB1 | 17 | 0.13 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB2 | 17 | 0.13 |
| (1,3013) | 1:217:A:GLY:H | 1:218:A:ALA:HB3 | 17 | 0.13 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 2 | 0.13 |
| (1,2915) | 1:167:A:ASP:H | 1:195:A:ASN:H | 10 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 6 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 6 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 8 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 8 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 13 | 0.13 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 13 | 0.13 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 11 | 0.13 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 6 | 0.13 |
| (1,2788) | 1:172:A:SER:H | 1:175:A:ASN:H | 5 | 0.13 |
| (1,2765) | 1:168:A:ALA:H | 1:196:A:ASN:HA | 1 | 0.13 |
| (1,2765) | 1:168:A:ALA:H | 1:196:A:ASN:HA | 6 | 0.13 |
| (1,2760) | 1:167:A:ASP:H | 1:195:A:ASN:HB2 | 4 | 0.13 |
| (1,2752) | 1:154:A:ILE:HA | 1:166:A:ASP:H | 4 | 0.13 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 3 | 0.13 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 11 | 0.13 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 15 | 0.13 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 20 | 0.13 |
| (1,2681) | 1:153:A:VAL:H | 1:166:A:ASP:HB3 | 4 | 0.13 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB1 | 5 | 0.13 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB2 | 5 | 0.13 |
| (1,2678) | 1:152:A:LYS:H | 1:168:A:ALA:HB3 | 5 | 0.13 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 17 | 0.13 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 17 | 0.13 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 7 | 0.13 |
| (1,2652) | 1:149:A:ALA:H | 1:179:A:LEU:HB3 | 5 | 0.13 |
| (1,2630) | 1:143:A:VAL:HG11 | 1:145:A:ALA:H | 12 | 0.13 |
| (1,2630) | 1:143:A:VAL:HG12 | 1:145:A:ALA:H | 12 | 0.13 |
| (1,2630) | 1:143:A:VAL:HG13 | 1:145:A:ALA:H | 12 | 0.13 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 8 | 0.13 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 1 | 0.13 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 1 | 0.13 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 1 | 0.13 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 4 | 0.13 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 4 | 0.13 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 4 | 0.13 |
| (1,2584) | 1:139:A:SER:H | 1:139:A:SER:HB2 | 2 | 0.13 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 9 | 0.13 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 11 | 0.13 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 18 | 0.13 |
| (1,2514) | 1:123:A:LYS:HG3 | 1:124:A:GLY:H | 5 | 0.13 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD11 | 7 | 0.13 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD12 | 7 | 0.13 |
| (1,2471) | 1:118:A:ILE:H | 1:118:A:ILE:HD13 | 7 | 0.13 |
| (1,2466) | 1:118:A:ILE:H | 1:140:A:ILE:HA | 8 | 0.13 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 19 | 0.13 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 19 | 0.13 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 19 | 0.13 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 16 | 0.13 |
| (1,2345) | 1:87:A:VAL:H | 1:87:A:VAL:HB | 17 | 0.13 |
| (1,2288) | 1:75:A:ILE:HB | 1:76:A:MET:H | 4 | 0.13 |
| (1,2273) | 1:74:A:ASP:H | 1:74:A:ASP:HB3 | 10 | 0.13 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 9 | 0.13 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 13 | 0.13 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 9 | 0.13 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 14 | 0.13 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 15 | 0.13 |
| (1,2136) | 1:101:A:VAL:HG11 | 1:102:A:ARG:HA | 4 | 0.13 |
| (1,2136) | 1:101:A:VAL:HG12 | 1:102:A:ARG:HA | 4 | 0.13 |
| (1,2136) | 1:101:A:VAL:HG13 | 1:102:A:ARG:HA | 4 | 0.13 |
| (1,2136) | 1:101:A:VAL:HG21 | 1:102:A:ARG:HA | 4 | 0.13 |
| (1,2136) | 1:101:A:VAL:HG22 | 1:102:A:ARG:HA | 4 | 0.13 |
| (1,2136) | 1:101:A:VAL:HG23 | 1:102:A:ARG:HA | 4 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD11 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD12 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG21 | 1:54:A:ILE:HD13 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD11 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD12 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG22 | 1:54:A:ILE:HD13 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD11 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD12 | 13 | 0.13 |
| (1,2119) | 1:52:A:VAL:HG23 | 1:54:A:ILE:HD13 | 13 | 0.13 |
| (1,2115) | 1:56:A:ALA:HB1 | 1:70:A:THR:HA | 10 | 0.13 |
| (1,2115) | 1:56:A:ALA:HB2 | 1:70:A:THR:HA | 10 | 0.13 |
| (1,2115) | 1:56:A:ALA:HB3 | 1:70:A:THR:HA | 10 | 0.13 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 14 | 0.13 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 14 | 0.13 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 14 | 0.13 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG21 | 13 | 0.13 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG22 | 13 | 0.13 |
| (1,2048) | 1:197:A:ALA:HA | 1:198:A:THR:HG23 | 13 | 0.13 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 1 | 0.13 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 18 | 0.13 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD21 | 15 | 0.13 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD22 | 15 | 0.13 |
| (1,2004) | 1:181:A:GLU:H | 1:216:A:LEU:HD23 | 15 | 0.13 |
| (1,1997) | 1:184:A:ILE:HA | 1:216:A:LEU:HB3 | 3 | 0.13 |
| (1,1963) | 1:161:A:LYS:HD2 | 1:189:A:VAL:H | 3 | 0.13 |
| (1,1963) | 1:161:A:LYS:HD3 | 1:189:A:VAL:H | 3 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 5 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 5 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 5 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 5 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 5 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 5 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 10 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 10 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 10 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 10 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 10 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 10 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 14 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 14 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 14 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 14 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 14 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 14 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 19 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 19 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 19 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 19 | 0.13 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 19 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 2 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 2 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 6 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 6 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 12 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 12 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 13 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 13 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 20 | 0.13 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 20 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 8 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 8 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 10 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 10 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 12 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 12 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 16 | 0.13 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 16 | 0.13 |
| (1,1867) | 1:166:A:ASP:HB2 | 1:195:A:ASN:H | 10 | 0.13 |
| (1,1866) | 1:165:A:PHE:H | 1:166:A:ASP:HB2 | 20 | 0.13 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 9 | 0.13 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 9 | 0.13 |
| (1,1812) | 1:201:A:ILE:HA | 1:205:A:LYS:H | 20 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 17 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 17 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 17 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 19 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 19 | 0.13 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 19 | 0.13 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 2 | 0.13 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 2 | 0.13 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 2 | 0.13 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 3 | 0.13 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 3 | 0.13 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 3 | 0.13 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 3 | 0.13 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 3 | 0.13 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 8 | 0.13 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 12 | 0.13 |
| (1,1722) | 1:195:A:ASN:HB3 | 1:196:A:ASN:HA | 4 | 0.13 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 1 | 0.13 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 12 | 0.13 |
| (1,1707) | 1:194:A:ILE:HG21 | 1:196:A:ASN:HA | 11 | 0.13 |
| (1,1707) | 1:194:A:ILE:HG22 | 1:196:A:ASN:HA | 11 | 0.13 |
| (1,1707) | 1:194:A:ILE:HG23 | 1:196:A:ASN:HA | 11 | 0.13 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD11 | 11 | 0.13 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD12 | 11 | 0.13 |
| (1,1698) | 1:165:A:PHE:HB2 | 1:194:A:ILE:HD13 | 11 | 0.13 |
| (1,1691) | 1:194:A:ILE:HD11 | 1:223:A:THR:H | 10 | 0.13 |
| (1,1691) | 1:194:A:ILE:HD12 | 1:223:A:THR:H | 10 | 0.13 |
| (1,1691) | 1:194:A:ILE:HD13 | 1:223:A:THR:H | 10 | 0.13 |
| (1,1647) | 1:191:A:THR:HA | 1:192:A:ILE:HB | 7 | 0.13 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 3 | 0.13 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 3 | 0.13 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 3 | 0.13 |
| (1,1621) | 1:162:A:THR:HG21 | 1:190:A:LYS:H | 9 | 0.13 |
| (1,1621) | 1:162:A:THR:HG22 | 1:190:A:LYS:H | 9 | 0.13 |
| (1,1621) | 1:162:A:THR:HG23 | 1:190:A:LYS:H | 9 | 0.13 |
| (1,1617) | 1:184:A:ILE:HG21 | 1:188:A:GLY:HA3 | 7 | 0.13 |
| (1,1617) | 1:184:A:ILE:HG22 | 1:188:A:GLY:HA3 | 7 | 0.13 |
| (1,1617) | 1:184:A:ILE:HG23 | 1:188:A:GLY:HA3 | 7 | 0.13 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 12 | 0.13 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 16 | 0.13 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 16 | 0.13 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 16 | 0.13 |
| (1,1602) | 1:142:A:THR:HG21 | 1:186:A:THR:HB | 20 | 0.13 |
| (1,1602) | 1:142:A:THR:HG22 | 1:186:A:THR:HB | 20 | 0.13 |
| (1,1602) | 1:142:A:THR:HG23 | 1:186:A:THR:HB | 20 | 0.13 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 3 | 0.13 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 4 | 0.13 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 7 | 0.13 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 10 | 0.13 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 18 | 0.13 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 20 | 0.13 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 17 | 0.13 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 17 | 0.13 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 18 | 0.13 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1582) | 1:201:A:ILE:HG21 | 1:205:A:LYS:HB3 | 3 | 0.13 |
| (1,1582) | 1:201:A:ILE:HG22 | 1:205:A:LYS:HB3 | 3 | 0.13 |
| (1,1582) | 1:201:A:ILE:HG23 | 1:205:A:LYS:HB3 | 3 | 0.13 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 18 | 0.13 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 18 | 0.13 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 18 | 0.13 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 17 | 0.13 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 17 | 0.13 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 17 | 0.13 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 6 | 0.13 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 6 | 0.13 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 16 | 0.13 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 16 | 0.13 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 3 | 0.13 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 3 | 0.13 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 3 | 0.13 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 1 | 0.13 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 1 | 0.13 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 1 | 0.13 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 1 | 0.13 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 1 | 0.13 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 1 | 0.13 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 1 | 0.13 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 12 | 0.13 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 2 | 0.13 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 10 | 0.13 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 10 | 0.13 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 10 | 0.13 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB1 | 20 | 0.13 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB2 | 20 | 0.13 |
| (1,1376) | 1:170:A:PHE:HA | 1:176:A:ALA:HB3 | 20 | 0.13 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 19 | 0.13 |
| (1,1360) | 1:153:A:VAL:HB | 1:166:A:ASP:HB2 | 12 | 0.13 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 11 | 0.13 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 3 | 0.13 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 3 | 0.13 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE1 | 6 | 0.13 |
| (1,1337) | 1:163:A:LEU:HB2 | 1:165:A:PHE:HE2 | 6 | 0.13 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE1 | 6 | 0.13 |
| (1,1337) | 1:163:A:LEU:HB3 | 1:165:A:PHE:HE2 | 6 | 0.13 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 8 | 0.13 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 8 | 0.13 |
| (1,1321) | 1:158:A:ASP:HB2 | 1:162:A:THR:HA | 7 | 0.13 |
| (1,1305) | 1:161:A:LYS:HD2 | 1:189:A:VAL:HA | 16 | 0.13 |
| (1,1305) | 1:161:A:LYS:HD3 | 1:189:A:VAL:HA | 16 | 0.13 |
| (1,1265) | 1:156:A:SER:H | 1:157:A:LEU:HA | 17 | 0.13 |
| (1,1264) | 1:157:A:LEU:HA | 1:159:A:ASN:HA | 13 | 0.13 |
| (1,1204) | 1:152:A:LYS:H | 1:152:A:LYS:HG3 | 11 | 0.13 |
| (1,1202) | 1:137:A:ASP:H | 1:152:A:LYS:HG2 | 9 | 0.13 |
| (1,1201) | 1:209:A:LEU:H | 1:210:A:LYS:HE2 | 15 | 0.13 |
| (1,1201) | 1:209:A:LEU:H | 1:210:A:LYS:HE3 | 15 | 0.13 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 13 | 0.13 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 15 | 0.13 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 5 | 0.13 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 5 | 0.13 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 5 | 0.13 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 13 | 0.13 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 13 | 0.13 |
| (1,1161) | 1:147:A:GLY:HA2 | 1:148:A:SER:HB2 | 3 | 0.13 |
| (1,1161) | 1:147:A:GLY:HA2 | 1:148:A:SER:HB3 | 3 | 0.13 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD11 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD12 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD13 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD21 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD22 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB2 | 1:179:A:LEU:HD23 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD11 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD12 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD13 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD21 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD22 | 5 | 0.13 |
| (1,1156) | 1:148:A:SER:HB3 | 1:179:A:LEU:HD23 | 5 | 0.13 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 13 | 0.13 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 7 | 0.13 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 7 | 0.13 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 7 | 0.13 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG2 | 3 | 0.13 |
| (1,1131) | 1:52:A:VAL:HG11 | 1:76:A:MET:HG3 | 3 | 0.13 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG2 | 3 | 0.13 |
| (1,1131) | 1:52:A:VAL:HG12 | 1:76:A:MET:HG3 | 3 | 0.13 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG2 | 3 | 0.13 |
| (1,1131) | 1:52:A:VAL:HG13 | 1:76:A:MET:HG3 | 3 | 0.13 |
| (1,1085) | 1:140:A:ILE:HD11 | 1:149:A:ALA:H | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1085) | 1:140:A:ILE:HD12 | 1:149:A:ALA:H | 18 | 0.13 |
| (1,1085) | 1:140:A:ILE:HD13 | 1:149:A:ALA:H | 18 | 0.13 |
| (1,1053) | 1:139:A:SER:HB3 | 1:140:A:ILE:H | 19 | 0.13 |
| (1,1049) | 1:120:A:LYS:HE2 | 1:139:A:SER:HB2 | 14 | 0.13 |
| (1,1049) | 1:120:A:LYS:HE3 | 1:139:A:SER:HB2 | 14 | 0.13 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 1 | 0.13 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 1 | 0.13 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 1 | 0.13 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 15 | 0.13 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 15 | 0.13 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 15 | 0.13 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 16 | 0.13 |
| (1,972) | 1:68:A:VAL:HA | 1:86:A:GLU:HG2 | 16 | 0.13 |
| (1,966) | 1:134:A:VAL:HA | 1:155:A:LYS:HG3 | 13 | 0.13 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG21 | 15 | 0.13 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG22 | 15 | 0.13 |
| (1,951) | 1:127:A:ASN:HD21 | 1:130:A:THR:HG23 | 15 | 0.13 |
| (1,949) | 1:130:A:THR:HB | 1:132:A:ASP:H | 20 | 0.13 |
| (1,938) | 1:103:A:THR:HA | 1:128:A:LEU:HG | 8 | 0.13 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 4 | 0.13 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 4 | 0.13 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 4 | 0.13 |
| (1,892) | 1:208:A:LYS:HD2 | 1:209:A:LEU:H | 10 | 0.13 |
| (1,892) | 1:208:A:LYS:HD3 | 1:209:A:LEU:H | 10 | 0.13 |
| (1,890) | 1:123:A:LYS:HD3 | 1:124:A:GLY:H | 5 | 0.13 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG11 | 12 | 0.13 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG12 | 12 | 0.13 |
| (1,829) | 1:116:A:GLN:H | 1:117:A:VAL:HG13 | 12 | 0.13 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 14 | 0.13 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 14 | 0.13 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 14 | 0.13 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 7 | 0.13 |
| (1,724) | 1:107:A:LEU:HD11 | 1:123:A:LYS:H | 19 | 0.13 |
| (1,724) | 1:107:A:LEU:HD12 | 1:123:A:LYS:H | 19 | 0.13 |
| (1,724) | 1:107:A:LEU:HD13 | 1:123:A:LYS:H | 19 | 0.13 |
| (1,724) | 1:107:A:LEU:HD21 | 1:123:A:LYS:H | 19 | 0.13 |
| (1,724) | 1:107:A:LEU:HD22 | 1:123:A:LYS:H | 19 | 0.13 |
| (1,724) | 1:107:A:LEU:HD23 | 1:123:A:LYS:H | 19 | 0.13 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB2 | 7 | 0.13 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB3 | 7 | 0.13 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 16 | 0.13 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG21 | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG22 | 18 | 0.13 |
| (1,701) | 1:129:A:ASN:HB3 | 1:130:A:THR:HG23 | 18 | 0.13 |
| (1,698) | 1:106:A:ALA:HB1 | 1:124:A:GLY:HA2 | 1 | 0.13 |
| (1,698) | 1:106:A:ALA:HB2 | 1:124:A:GLY:HA2 | 1 | 0.13 |
| (1,698) | 1:106:A:ALA:HB3 | 1:124:A:GLY:HA2 | 1 | 0.13 |
| (1,621) | 1:94:A:ALA:HB1 | 1:98:A:PRO:HD2 | 9 | 0.13 |
| (1,621) | 1:94:A:ALA:HB2 | 1:98:A:PRO:HD2 | 9 | 0.13 |
| (1,621) | 1:94:A:ALA:HB3 | 1:98:A:PRO:HD2 | 9 | 0.13 |
| (1,619) | 1:98:A:PRO:HB2 | 1:99:A:GLU:HA | 14 | 0.13 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 8 | 0.13 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 8 | 0.13 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 2 | 0.13 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 2 | 0.13 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 2 | 0.13 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 10 | 0.13 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 10 | 0.13 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 10 | 0.13 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 10 | 0.13 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 10 | 0.13 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 10 | 0.13 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 6 | 0.13 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 6 | 0.13 |
| (1,492) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HG2 | 7 | 0.13 |
| (1,492) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HG2 | 7 | 0.13 |
| (1,485) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HA | 10 | 0.13 |
| (1,484) | 1:82:A:LEU:HG | 1:83:A:GLN:H | 6 | 0.13 |
| (1,444) | 1:77:A:GLN:HA | 1:78:A:GLY:HA3 | 9 | 0.13 |
| (1,444) | 1:77:A:GLN:HA | 1:78:A:GLY:HA3 | 12 | 0.13 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 4 | 0.13 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 4 | 0.13 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 4 | 0.13 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB2 | 3 | 0.13 |
| (1,439) | 1:141:A:GLU:HB3 | 1:148:A:SER:HB3 | 3 | 0.13 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 17 | 0.13 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 17 | 0.13 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 17 | 0.13 |
| (1,371) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HA | 19 | 0.13 |
| (1,354) | 1:73:A:VAL:HG11 | 1:86:A:GLU:HA | 18 | 0.13 |
| (1,354) | 1:73:A:VAL:HG12 | 1:86:A:GLU:HA | 18 | 0.13 |
| (1,354) | 1:73:A:VAL:HG13 | 1:86:A:GLU:HA | 18 | 0.13 |
| (1,353) | 1:73:A:VAL:HG11 | 1:74:A:ASP:HA | 19 | 0.13 |
| (1,353) | 1:73:A:VAL:HG12 | 1:74:A:ASP:HA | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,353) | 1:73:A:VAL:HG13 | 1:74:A:ASP:HA | 19 | 0.13 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 15 | 0.13 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 12 | 0.13 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 12 | 0.13 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 12 | 0.13 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 8 | 0.13 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 10 | 0.13 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 10 | 0.13 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 10 | 0.13 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 12 | 0.13 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 12 | 0.13 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 12 | 0.13 |
| (1,170) | 1:56:A:ALA:HB1 | 1:69:A:PHE:H | 8 | 0.13 |
| (1,170) | 1:56:A:ALA:HB2 | 1:69:A:PHE:H | 8 | 0.13 |
| (1,170) | 1:56:A:ALA:HB3 | 1:69:A:PHE:H | 8 | 0.13 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 12 | 0.13 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 12 | 0.13 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 12 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 17 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 18 | 0.13 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 18 | 0.13 |
| (1,80) | 1:53:A:THR:HA | 2:9:B:ILE:HA | 14 | 0.13 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 7 | 0.13 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 9 | 0.13 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 7 | 0.13 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 10 | 0.13 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 18 | 0.13 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG21 | 9 | 0.13 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG22 | 9 | 0.13 |
| (1,36) | 1:51:A:PRO:HA | 2:8:B:ILE:HG23 | 9 | 0.13 |
| (1,35) | 1:155:A:LYS:HB3 | 1:155:A:LYS:HE2 | 13 | 0.13 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 9 | 0.12 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 9 | 0.12 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 14 | 0.12 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 14 | 0.12 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB2 | 6 | 0.12 |
| (1,4007) | 2:9:B:ILE:HD11 | 2:20:B:ARG:HB3 | 6 | 0.12 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB2 | 6 | 0.12 |
| (1,4007) | 2:9:B:ILE:HD12 | 2:20:B:ARG:HB3 | 6 | 0.12 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB2 | 6 | 0.12 |
| (1,4007) | 2:9:B:ILE:HD13 | 2:20:B:ARG:HB3 | 6 | 0.12 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 7 | 0.12 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 7 | 0.12 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 7 | 0.12 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 7 | 0.12 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 7 | 0.12 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 7 | 0.12 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 17 | 0.12 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 17 | 0.12 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 17 | 0.12 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 17 | 0.12 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 17 | 0.12 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 17 | 0.12 |
| (1,3904) | 1:177:A:GLU:HG2 | 1:209:A:LEU:HA | 6 | 0.12 |
| (1,3904) | 1:177:A:GLU:HG3 | 1:209:A:LEU:HA | 6 | 0.12 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB2 | 17 | 0.12 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB3 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 17 | 0.12 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 17 | 0.12 |
| (1,3753) | 1:112:A:TYR:H | 1:120:A:LYS:HD2 | 12 | 0.12 |
| (1,3753) | 1:112:A:TYR:H | 1:120:A:LYS:HD3 | 12 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG11 | 1:123:A:LYS:H | 1 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG12 | 1:123:A:LYS:H | 1 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG13 | 1:123:A:LYS:H | 1 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG21 | 1:123:A:LYS:H | 1 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG22 | 1:123:A:LYS:H | 1 | 0.12 |
| (1,3740) | 1:110:A:VAL:HG23 | 1:123:A:LYS:H | 1 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 3 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 3 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 3 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 3 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 3 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 3 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 8 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 8 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 8 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 8 | 0.12 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 8 | 0.12 |
| (1,3707) | 1:102:A:ARG:HG2 | 1:103:A:THR:H | 18 | 0.12 |
| (1,3707) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 18 | 0.12 |
| (1,3703) | 1:102:A:ARG:H | 1:129:A:ASN:HD21 | 6 | 0.12 |
| (1,3703) | 1:102:A:ARG:H | 1:129:A:ASN:HD22 | 6 | 0.12 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE21 | 16 | 0.12 |
| (1,3671) | 1:91:A:GLN:HB2 | 1:91:A:GLN:HE22 | 16 | 0.12 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE21 | 16 | 0.12 |
| (1,3671) | 1:91:A:GLN:HB3 | 1:91:A:GLN:HE22 | 16 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 14 | 0.12 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 14 | 0.12 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB2 | 7 | 0.12 |
| (1,3606) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HB3 | 7 | 0.12 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB2 | 7 | 0.12 |
| (1,3606) | 1:77:A:GLN:HE22 | 1:128:A:LEU:HB3 | 7 | 0.12 |
| (1,3590) | 1:74:A:ASP:HB2 | 1:83:A:GLN:HG3 | 15 | 0.12 |
| (1,3590) | 1:74:A:ASP:HB3 | 1:83:A:GLN:HG3 | 15 | 0.12 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB2 | 5 | 0.12 |
| (1,3555) | 1:56:A:ALA:HA | 1:74:A:ASP:HB3 | 5 | 0.12 |
| (1,3504) | 1:52:A:VAL:HB | 2:8:B:ILE:HA | 20 | 0.12 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD1 | 4 | 0.12 |
| (1,3495) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HD2 | 4 | 0.12 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD1 | 4 | 0.12 |
| (1,3495) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HD2 | 4 | 0.12 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD1 | 4 | 0.12 |
| (1,3495) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HD2 | 4 | 0.12 |
| (1,3489) | 1:54:A:ILE:HD11 | 2:8:B:ILE:HG12 | 10 | 0.12 |
| (1,3489) | 1:54:A:ILE:HD12 | 2:8:B:ILE:HG12 | 10 | 0.12 |
| (1,3489) | 1:54:A:ILE:HD13 | 2:8:B:ILE:HG12 | 10 | 0.12 |
| (1,3483) | 1:53:A:THR:HG21 | 2:9:B:ILE:H | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3483) | 1:53:A:THR:HG22 | 2:9:B:ILE:H | 1 | 0.12 |
| (1,3483) | 1:53:A:THR:HG23 | 2:9:B:ILE:H | 1 | 0.12 |
| (1,3482) | 1:53:A:THR:HG21 | 2:10:B:TYR:HA | 17 | 0.12 |
| (1,3482) | 1:53:A:THR:HG22 | 2:10:B:TYR:HA | 17 | 0.12 |
| (1,3482) | 1:53:A:THR:HG23 | 2:10:B:TYR:HA | 17 | 0.12 |
| (1,3475) | 2:10:B:TYR:HD1 | 2:21:B:MET:HB3 | 4 | 0.12 |
| (1,3475) | 2:10:B:TYR:HD2 | 2:21:B:MET:HB3 | 4 | 0.12 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE1 | 10 | 0.12 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE2 | 10 | 0.12 |
| (1,3467) | 2:21:B:MET:HB2 | 2:21:B:MET:HE3 | 10 | 0.12 |
| (1,3437) | 2:12:B:ASN:HB2 | 2:16:B:GLY:H | 20 | 0.12 |
| (1,3340) | 2:13:B:ARG:HA | 2:15:B:THR:H | 18 | 0.12 |
| (1,3332) | 2:13:B:ARG:H | 2:14:B:ARG:HA | 7 | 0.12 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD2 | 2 | 0.12 |
| (1,3328) | 2:9:B:ILE:H | 2:20:B:ARG:HD3 | 2 | 0.12 |
| (1,3289) | 2:4:B:LYS:HB2 | 2:5:B:PRO:HD3 | 16 | 0.12 |
| (1,3289) | 2:4:B:LYS:HB3 | 2:5:B:PRO:HD3 | 16 | 0.12 |
| (1,3272) | 1:111:A:HIS:HB3 | 1:111:A:HIS:HD2 | 14 | 0.12 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB1 | 4 | 0.12 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB2 | 4 | 0.12 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB3 | 4 | 0.12 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 19 | 0.12 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 19 | 0.12 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 19 | 0.12 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 19 | 0.12 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 19 | 0.12 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 19 | 0.12 |
| (1,3156) | 1:125:A:TRP:H | 1:135:A:PHE:HD1 | 16 | 0.12 |
| (1,3156) | 1:125:A:TRP:H | 1:135:A:PHE:HD2 | 16 | 0.12 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG11 | 18 | 0.12 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG12 | 18 | 0.12 |
| (1,3154) | 1:69:A:PHE:HD1 | 1:73:A:VAL:HG13 | 18 | 0.12 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG11 | 18 | 0.12 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG12 | 18 | 0.12 |
| (1,3154) | 1:69:A:PHE:HD2 | 1:73:A:VAL:HG13 | 18 | 0.12 |
| (1,3145) | 1:173:A:TYR:HD1 | 1:205:A:LYS:HB2 | 11 | 0.12 |
| (1,3145) | 1:173:A:TYR:HD2 | 1:205:A:LYS:HB2 | 11 | 0.12 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 10 | 0.12 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 10 | 0.12 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 10 | 0.12 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 10 | 0.12 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 10 | 0.12 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 14 | 0.12 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 14 | 0.12 |
| (1,3094) | 1:54:A:ILE:H | 1:76:A:MET:HB2 | 15 | 0.12 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD11 | 18 | 0.12 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD12 | 18 | 0.12 |
| (1,3093) | 1:50:A:LEU:H | 1:50:A:LEU:HD13 | 18 | 0.12 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 18 | 0.12 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 18 | 0.12 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 18 | 0.12 |
| (1,3048) | 1:196:A:ASN:HA | 1:225:A:LYS:H | 9 | 0.12 |
| (1,3032) | 1:191:A:THR:HA | 1:220:A:LEU:H | 12 | 0.12 |
| (1,3028) | 1:190:A:LYS:HG3 | 1:219:A:THR:H | 12 | 0.12 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 4 | 0.12 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 7 | 0.12 |
| (1,3023) | 1:191:A:THR:H | 1:219:A:THR:H | 4 | 0.12 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 5 | 0.12 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 5 | 0.12 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD11 | 14 | 0.12 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD12 | 14 | 0.12 |
| (1,2938) | 1:197:A:ALA:H | 1:222:A:ILE:HD13 | 14 | 0.12 |
| (1,2927) | 1:195:A:ASN:HB2 | 1:196:A:ASN:H | 13 | 0.12 |
| (1,2920) | 1:166:A:ASP:HA | 1:195:A:ASN:H | 11 | 0.12 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 4 | 0.12 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 19 | 0.12 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 19 | 0.12 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 20 | 0.12 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 2 | 0.12 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 2 | 0.12 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 2 | 0.12 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 14 | 0.12 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 14 | 0.12 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 14 | 0.12 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 8 | 0.12 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE1 | 1 | 0.12 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE2 | 1 | 0.12 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE1 | 13 | 0.12 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE2 | 13 | 0.12 |
| (1,2767) | 1:168:A:ALA:H | 1:196:A:ASN:HD21 | 1 | 0.12 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 9 | 0.12 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 14 | 0.12 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 14 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 14 | 0.12 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 14 | 0.12 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 14 | 0.12 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 14 | 0.12 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 14 | 0.12 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD21 | 4 | 0.12 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD22 | 4 | 0.12 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD23 | 4 | 0.12 |
| (1,2711) | 1:157:A:LEU:H | 1:162:A:THR:HB | 13 | 0.12 |
| (1,2709) | 1:156:A:SER:H | 1:157:A:LEU:H | 19 | 0.12 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 12 | 0.12 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 13 | 0.12 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 12 | 0.12 |
| (1,2627) | 1:142:A:THR:HB | 1:145:A:ALA:H | 15 | 0.12 |
| (1,2611) | 1:116:A:GLN:H | 1:143:A:VAL:H | 5 | 0.12 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 2 | 0.12 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 2 | 0.12 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 2 | 0.12 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 17 | 0.12 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 17 | 0.12 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 17 | 0.12 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 2 | 0.12 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 17 | 0.12 |
| (1,2605) | 1:142:A:THR:H | 1:148:A:SER:HA | 20 | 0.12 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 14 | 0.12 |
| (1,2544) | 1:128:A:LEU:HD11 | 1:131:A:LYS:H | 7 | 0.12 |
| (1,2544) | 1:128:A:LEU:HD12 | 1:131:A:LYS:H | 7 | 0.12 |
| (1,2544) | 1:128:A:LEU:HD13 | 1:131:A:LYS:H | 7 | 0.12 |
| (1,2544) | 1:128:A:LEU:HD21 | 1:131:A:LYS:H | 7 | 0.12 |
| (1,2544) | 1:128:A:LEU:HD22 | 1:131:A:LYS:H | 7 | 0.12 |
| (1,2544) | 1:128:A:LEU:HD23 | 1:131:A:LYS:H | 7 | 0.12 |
| (1,2393) | 1:102:A:ARG:HG3 | 1:103:A:THR:H | 6 | 0.12 |
| (1,2379) | 1:94:A:ALA:HB1 | 1:97:A:GLN:H | 17 | 0.12 |
| (1,2379) | 1:94:A:ALA:HB2 | 1:97:A:GLN:H | 17 | 0.12 |
| (1,2379) | 1:94:A:ALA:HB3 | 1:97:A:GLN:H | 17 | 0.12 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 4 | 0.12 |
| (1,2369) | 1:163:A:LEU:HG | 1:164:A:GLU:H | 10 | 0.12 |
| (1,2344) | 1:86:A:GLU:HG2 | 1:87:A:VAL:H | 1 | 0.12 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD1 | 20 | 0.12 |
| (1,2312) | 1:83:A:GLN:H | 1:112:A:TYR:HD2 | 20 | 0.12 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 19 | 0.12 |
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE1 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2300) | 1:80:A:SER:H | 1:112:A:TYR:HE2 | 20 | 0.12 |
| (1,2294) | 1:76:A:MET:HB3 | 1:77:A:GLN:H | 1 | 0.12 |
| (1,2288) | 1:75:A:ILE:HB | 1:76:A:MET:H | 17 | 0.12 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 1 | 0.12 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 3 | 0.12 |
| (1,2197) | 1:59:A:ALA:H | 2:12:B:ASN:HD22 | 6 | 0.12 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 1 | 0.12 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 3 | 0.12 |
| (1,2196) | 1:58:A:HIS:HE1 | 1:59:A:ALA:H | 13 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG11 | 1:102:A:ARG:HA | 14 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG12 | 1:102:A:ARG:HA | 14 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG13 | 1:102:A:ARG:HA | 14 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG21 | 1:102:A:ARG:HA | 14 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG22 | 1:102:A:ARG:HA | 14 | 0.12 |
| (1,2136) | 1:101:A:VAL:HG23 | 1:102:A:ARG:HA | 14 | 0.12 |
| (1,2129) | 1:80:A:SER:HB3 | 1:114:A:ASP:HB3 | 9 | 0.12 |
| (1,2120) | 1:74:A:ASP:HA | 1:83:A:GLN:HG3 | 10 | 0.12 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 5 | 0.12 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 5 | 0.12 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 5 | 0.12 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG21 | 14 | 0.12 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG22 | 14 | 0.12 |
| (1,2025) | 1:190:A:LYS:HB3 | 1:219:A:THR:HG23 | 14 | 0.12 |
| (1,2023) | 1:190:A:LYS:HG3 | 1:219:A:THR:HB | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 1 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 1 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 1 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 1 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 1 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 1 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 4 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 6 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 6 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 6 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 6 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 6 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 7 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 7 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 7 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 7 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 7 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 7 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 12 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 12 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 12 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 12 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 12 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 12 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 17 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 17 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 17 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 17 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 17 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 17 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 20 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 20 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 20 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 20 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 20 | 0.12 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 20 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 10 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 10 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 14 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 14 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 18 | 0.12 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 18 | 0.12 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 4 | 0.12 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 4 | 0.12 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 10 | 0.12 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 16 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 10 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 10 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 10 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 12 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 12 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 12 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 18 | 0.12 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 18 | 0.12 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 15 | 0.12 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 15 | 0.12 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 15 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 7 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 7 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 7 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 20 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 20 | 0.12 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 20 | 0.12 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 7 | 0.12 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 7 | 0.12 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 7 | 0.12 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 1 | 0.12 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 16 | 0.12 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 1 | 0.12 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 1 | 0.12 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 1 | 0.12 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 15 | 0.12 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 7 | 0.12 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 13 | 0.12 |
| (1,1725) | 1:196:A:ASN:HA | 1:225:A:LYS:HB2 | 12 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB1 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB2 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD11 | 1:197:A:ALA:HB3 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB1 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB2 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD12 | 1:197:A:ALA:HB3 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB1 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB2 | 17 | 0.12 |
| (1,1701) | 1:194:A:ILE:HD13 | 1:197:A:ALA:HB3 | 17 | 0.12 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 17 | 0.12 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 17 | 0.12 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 17 | 0.12 |
| (1,1674) | 1:192:A:ILE:HG21 | 1:193:A:THR:HB | 16 | 0.12 |
| (1,1674) | 1:192:A:ILE:HG22 | 1:193:A:THR:HB | 16 | 0.12 |
| (1,1674) | 1:192:A:ILE:HG23 | 1:193:A:THR:HB | 16 | 0.12 |
| (1,1656) | 1:192:A:ILE:HD11 | 1:220:A:LEU:H | 3 | 0.12 |
| (1,1656) | 1:192:A:ILE:HD12 | 1:220:A:LEU:H | 3 | 0.12 |
| (1,1656) | 1:192:A:ILE:HD13 | 1:220:A:LEU:H | 3 | 0.12 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD2 | 15 | 0.12 |
| (1,1626) | 1:190:A:LYS:HA | 1:190:A:LYS:HD3 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 6 | 0.12 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 6 | 0.12 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 6 | 0.12 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 2 | 0.12 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 8 | 0.12 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 17 | 0.12 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 6 | 0.12 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 6 | 0.12 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 6 | 0.12 |
| (1,1599) | 1:185:A:LYS:H | 1:186:A:THR:HB | 11 | 0.12 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 6 | 0.12 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 6 | 0.12 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 14 | 0.12 |
| (1,1580) | 1:208:A:LYS:HA | 1:211:A:ALA:H | 5 | 0.12 |
| (1,1570) | 1:184:A:ILE:HG21 | 1:216:A:LEU:HA | 4 | 0.12 |
| (1,1570) | 1:184:A:ILE:HG22 | 1:216:A:LEU:HA | 4 | 0.12 |
| (1,1570) | 1:184:A:ILE:HG23 | 1:216:A:LEU:HA | 4 | 0.12 |
| (1,1567) | 1:184:A:ILE:HG21 | 1:189:A:VAL:H | 19 | 0.12 |
| (1,1567) | 1:184:A:ILE:HG22 | 1:189:A:VAL:H | 19 | 0.12 |
| (1,1567) | 1:184:A:ILE:HG23 | 1:189:A:VAL:H | 19 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD11 | 1:219:A:THR:H | 5 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD12 | 1:219:A:THR:H | 5 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD13 | 1:219:A:THR:H | 5 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD11 | 1:219:A:THR:H | 20 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD12 | 1:219:A:THR:H | 20 | 0.12 |
| (1,1549) | 1:184:A:ILE:HD13 | 1:219:A:THR:H | 20 | 0.12 |
| (1,1542) | 1:184:A:ILE:HA | 1:189:A:VAL:HB | 11 | 0.12 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 14 | 0.12 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 14 | 0.12 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 14 | 0.12 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 20 | 0.12 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 20 | 0.12 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 20 | 0.12 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 20 | 0.12 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 20 | 0.12 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 20 | 0.12 |
| (1,1521) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HA | 5 | 0.12 |
| (1,1521) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HA | 5 | 0.12 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 8 | 0.12 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 8 | 0.12 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 15 | 0.12 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 15 | 0.12 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 19 | 0.12 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 19 | 0.12 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 19 | 0.12 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 20 | 0.12 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 20 | 0.12 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 20 | 0.12 |
| (1,1484) | 1:180:A:ILE:HB | 1:181:A:GLU:H | 3 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD11 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD12 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD11 | 1:194:A:ILE:HD13 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD11 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD12 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD12 | 1:194:A:ILE:HD13 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD11 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD12 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD13 | 1:194:A:ILE:HD13 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD11 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD12 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD21 | 1:194:A:ILE:HD13 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD11 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD12 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD22 | 1:194:A:ILE:HD13 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD11 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD12 | 2 | 0.12 |
| (1,1481) | 1:179:A:LEU:HD23 | 1:194:A:ILE:HD13 | 2 | 0.12 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 8 | 0.12 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 8 | 0.12 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 8 | 0.12 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 8 | 0.12 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 8 | 0.12 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 8 | 0.12 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 13 | 0.12 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 15 | 0.12 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 4 | 0.12 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 7 | 0.12 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 11 | 0.12 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 16 | 0.12 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 17 | 0.12 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 5 | 0.12 |
| (1,1396) | 1:173:A:TYR:HB2 | 1:174:A:GLU:HA | 14 | 0.12 |
| (1,1372) | 1:168:A:ALA:HA | 1:169:A:THR:HB | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1360) | 1:153:A:VAL:HB | 1:166:A:ASP:HB2 | 9 | 0.12 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB1 | 15 | 0.12 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB2 | 15 | 0.12 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB3 | 15 | 0.12 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD11 | 15 | 0.12 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD12 | 15 | 0.12 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD13 | 15 | 0.12 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD21 | 15 | 0.12 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD22 | 15 | 0.12 |
| (1,1343) | 1:156:A:SER:HA | 1:163:A:LEU:HD23 | 15 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 8 | 0.12 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 8 | 0.12 |
| (1,1335) | 1:162:A:THR:HG21 | 1:164:A:GLU:H | 2 | 0.12 |
| (1,1335) | 1:162:A:THR:HG22 | 1:164:A:GLU:H | 2 | 0.12 |
| (1,1335) | 1:162:A:THR:HG23 | 1:164:A:GLU:H | 2 | 0.12 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG21 | 5 | 0.12 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG22 | 5 | 0.12 |
| (1,1331) | 1:158:A:ASP:HB2 | 1:162:A:THR:HG23 | 5 | 0.12 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 14 | 0.12 |
| (1,1302) | 1:161:A:LYS:HD2 | 1:190:A:LYS:H | 9 | 0.12 |
| (1,1302) | 1:161:A:LYS:HD3 | 1:190:A:LYS:H | 9 | 0.12 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 7 | 0.12 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 8 | 0.12 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 15 | 0.12 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 20 | 0.12 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD21 | 12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD22 | 12 | 0.12 |
| (1,1245) | 1:155:A:LYS:HB2 | 1:157:A:LEU:HD23 | 12 | 0.12 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG21 | 12 | 0.12 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG22 | 12 | 0.12 |
| (1,1241) | 1:133:A:TRP:HH2 | 1:154:A:ILE:HG23 | 12 | 0.12 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG21 | 5 | 0.12 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG22 | 5 | 0.12 |
| (1,1236) | 1:135:A:PHE:H | 1:154:A:ILE:HG23 | 5 | 0.12 |
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 8 | 0.12 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 8 | 0.12 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 8 | 0.12 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 11 | 0.12 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 11 | 0.12 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 11 | 0.12 |
| (1,1204) | 1:152:A:LYS:H | 1:152:A:LYS:HG3 | 9 | 0.12 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 13 | 0.12 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 7 | 0.12 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 7 | 0.12 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 19 | 0.12 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 15 | 0.12 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 15 | 0.12 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 15 | 0.12 |
| (1,1137) | 1:145:A:ALA:HB1 | 1:182:A:HIS:HB2 | 17 | 0.12 |
| (1,1137) | 1:145:A:ALA:HB2 | 1:182:A:HIS:HB2 | 17 | 0.12 |
| (1,1137) | 1:145:A:ALA:HB3 | 1:182:A:HIS:HB2 | 17 | 0.12 |
| (1,1129) | 1:118:A:ILE:HG13 | 1:143:A:VAL:HB | 19 | 0.12 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 7 | 0.12 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 7 | 0.12 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 7 | 0.12 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 18 | 0.12 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 18 | 0.12 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 18 | 0.12 |
| (1,1097) | 1:140:A:ILE:HG21 | 1:151:A:ALA:H | 16 | 0.12 |
| (1,1097) | 1:140:A:ILE:HG22 | 1:151:A:ALA:H | 16 | 0.12 |
| (1,1097) | 1:140:A:ILE:HG23 | 1:151:A:ALA:H | 16 | 0.12 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE1 | 4 | 0.12 |
| (1,1081) | 1:140:A:ILE:HD11 | 1:165:A:PHE:HE2 | 4 | 0.12 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE1 | 4 | 0.12 |
| (1,1081) | 1:140:A:ILE:HD12 | 1:165:A:PHE:HE2 | 4 | 0.12 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE1 | 4 | 0.12 |
| (1,1081) | 1:140:A:ILE:HD13 | 1:165:A:PHE:HE2 | 4 | 0.12 |
| (1,1076) | 1:140:A:ILE:HD11 | 1:142:A:THR:HA | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1076) | 1:140:A:ILE:HD12 | 1:142:A:THR:HA | 20 | 0.12 |
| (1,1076) | 1:140:A:ILE:HD13 | 1:142:A:THR:HA | 20 | 0.12 |
| (1,1068) | 1:50:A:LEU:HB2 | 1:51:A:PRO:HD3 | 18 | 0.12 |
| (1,1061) | 1:117:A:VAL:HB | 1:140:A:ILE:HA | 19 | 0.12 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 3 | 0.12 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 3 | 0.12 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 3 | 0.12 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG21 | 8 | 0.12 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG22 | 8 | 0.12 |
| (1,1044) | 1:139:A:SER:HB3 | 1:140:A:ILE:HG23 | 8 | 0.12 |
| (1,1006) | 1:136:A:TYR:HB3 | 1:152:A:LYS:HA | 6 | 0.12 |
| (1,1002) | 1:123:A:LYS:HD3 | 1:136:A:TYR:HB3 | 6 | 0.12 |
| (1,966) | 1:134:A:VAL:HA | 1:155:A:LYS:HG3 | 9 | 0.12 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG2 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD11 | 1:131:A:LYS:HG3 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG2 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD12 | 1:131:A:LYS:HG3 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG2 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD13 | 1:131:A:LYS:HG3 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG2 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD21 | 1:131:A:LYS:HG3 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG2 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD22 | 1:131:A:LYS:HG3 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG2 | 3 | 0.12 |
| (1,962) | 1:128:A:LEU:HD23 | 1:131:A:LYS:HG3 | 3 | 0.12 |
| (1,950) | 1:130:A:THR:HB | 1:131:A:LYS:H | 1 | 0.12 |
| (1,915) | 1:125:A:TRP:HB2 | 1:134:A:VAL:HB | 9 | 0.12 |
| (1,911) | 1:125:A:TRP:HA | 1:134:A:VAL:HB | 2 | 0.12 |
| (1,900) | 1:153:A:VAL:HG11 | 1:155:A:LYS:HE3 | 7 | 0.12 |
| (1,900) | 1:153:A:VAL:HG12 | 1:155:A:LYS:HE3 | 7 | 0.12 |
| (1,900) | 1:153:A:VAL:HG13 | 1:155:A:LYS:HE3 | 7 | 0.12 |
| (1,893) | 1:155:A:LYS:HE3 | 1:166:A:ASP:H | 12 | 0.12 |
| (1,879) | 1:107:A:LEU:HA | 1:123:A:LYS:HB2 | 7 | 0.12 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 3 | 0.12 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 3 | 0.12 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 3 | 0.12 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 9 | 0.12 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 9 | 0.12 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 9 | 0.12 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 1 | 0.12 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 1 | 0.12 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 1 | 0.12 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 1 | 0.12 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 1 | 0.12 |
| (1,822) | 1:117:A:VAL:HG11 | 1:133:A:TRP:HZ2 | 4 | 0.12 |
| (1,822) | 1:117:A:VAL:HG12 | 1:133:A:TRP:HZ2 | 4 | 0.12 |
| (1,822) | 1:117:A:VAL:HG13 | 1:133:A:TRP:HZ2 | 4 | 0.12 |
| (1,808) | 1:116:A:GLN:H | 1:117:A:VAL:HA | 2 | 0.12 |
| (1,805) | 1:117:A:VAL:HA | 1:143:A:VAL:HB | 18 | 0.12 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 5 | 0.12 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 5 | 0.12 |
| (1,784) | 1:115:A:ASN:HA | 1:143:A:VAL:HB | 2 | 0.12 |
| (1,776) | 1:113:A:ASP:HA | 1:118:A:ILE:HG12 | 11 | 0.12 |
| (1,764) | 1:84:A:ALA:HA | 1:111:A:HIS:HB2 | 17 | 0.12 |
| (1,735) | 1:108:A:GLY:H | 1:109:A:ASN:HA | 2 | 0.12 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 1 | 0.12 |
| (1,710) | 1:107:A:LEU:HA | 1:123:A:LYS:HD3 | 9 | 0.12 |
| (1,698) | 1:106:A:ALA:HB1 | 1:124:A:GLY:HA2 | 2 | 0.12 |
| (1,698) | 1:106:A:ALA:HB2 | 1:124:A:GLY:HA2 | 2 | 0.12 |
| (1,698) | 1:106:A:ALA:HB3 | 1:124:A:GLY:HA2 | 2 | 0.12 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG21 | 4 | 0.12 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG22 | 4 | 0.12 |
| (1,687) | 1:164:A:GLU:HA | 1:193:A:THR:HG23 | 4 | 0.12 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 5 | 0.12 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 9 | 0.12 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 20 | 0.12 |
| (1,676) | 1:103:A:THR:HG21 | 1:128:A:LEU:H | 7 | 0.12 |
| (1,676) | 1:103:A:THR:HG22 | 1:128:A:LEU:H | 7 | 0.12 |
| (1,676) | 1:103:A:THR:HG23 | 1:128:A:LEU:H | 7 | 0.12 |
| (1,639) | 1:101:A:VAL:HA | 1:103:A:THR:HG21 | 10 | 0.12 |
| (1,639) | 1:101:A:VAL:HA | 1:103:A:THR:HG22 | 10 | 0.12 |
| (1,639) | 1:101:A:VAL:HA | 1:103:A:THR:HG23 | 10 | 0.12 |
| (1,619) | 1:98:A:PRO:HB2 | 1:99:A:GLU:HA | 10 | 0.12 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 1 | 0.12 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 1 | 0.12 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 5 | 0.12 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 5 | 0.12 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 14 | 0.12 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 14 | 0.12 |
| (1,601) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HB3 | 16 | 0.12 |
| (1,601) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HB3 | 16 | 0.12 |
| (1,601) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HB3 | 16 | 0.12 |
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG2 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,597) | 1:118:A:ILE:H | 1:141:A:GLU:HG3 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 6 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 20 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 20 | 0.12 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 20 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 20 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 20 | 0.12 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 20 | 0.12 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG2 | 9 | 0.12 |
| (1,578) | 1:91:A:GLN:H | 1:92:A:LYS:HG3 | 9 | 0.12 |
| (1,564) | 1:74:A:ASP:HA | 1:75:A:ILE:HB | 12 | 0.12 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB1 | 19 | 0.12 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB2 | 19 | 0.12 |
| (1,563) | 1:119:A:LEU:HA | 1:138:A:ALA:HB3 | 19 | 0.12 |
| (1,535) | 1:99:A:GLU:HB3 | 1:100:A:PRO:HD3 | 5 | 0.12 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 18 | 0.12 |
| (1,446) | 1:50:A:LEU:HD11 | 1:78:A:GLY:HA3 | 7 | 0.12 |
| (1,446) | 1:50:A:LEU:HD12 | 1:78:A:GLY:HA3 | 7 | 0.12 |
| (1,446) | 1:50:A:LEU:HD13 | 1:78:A:GLY:HA3 | 7 | 0.12 |
| (1,441) | 1:77:A:GLN:HG3 | 1:128:A:LEU:HD11 | 3 | 0.12 |
| (1,441) | 1:77:A:GLN:HG3 | 1:128:A:LEU:HD12 | 3 | 0.12 |
| (1,441) | 1:77:A:GLN:HG3 | 1:128:A:LEU:HD13 | 3 | 0.12 |
| (1,441) | 1:77:A:GLN:HG3 | 1:128:A:LEU:HD21 | 3 | 0.12 |
| (1,441) | 1:77:A:GLN:HG3 | 1:128:A:LEU:HD22 | 3 | 0.12 |
| (1,441) | 1:77:A:GLN:HG3 | 1:128:A:LEU:HD23 | 3 | 0.12 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG2 | 18 | 0.12 |
| (1,431) | 1:55:A:ASN:HD22 | 1:76:A:MET:HG3 | 18 | 0.12 |
| (1,421) | 1:75:A:ILE:HG21 | 1:76:A:MET:HB3 | 3 | 0.12 |
| (1,421) | 1:75:A:ILE:HG22 | 1:76:A:MET:HB3 | 3 | 0.12 |
| (1,421) | 1:75:A:ILE:HG23 | 1:76:A:MET:HB3 | 3 | 0.12 |
| (1,409) | 1:75:A:ILE:HG21 | 1:76:A:MET:HA | 7 | 0.12 |
| (1,409) | 1:75:A:ILE:HG22 | 1:76:A:MET:HA | 7 | 0.12 |
| (1,409) | 1:75:A:ILE:HG23 | 1:76:A:MET:HA | 7 | 0.12 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD11 | 14 | 0.12 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD12 | 14 | 0.12 |
| (1,385) | 1:170:A:PHE:HE1 | 1:222:A:ILE:HD13 | 14 | 0.12 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD11 | 14 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD12 | 14 | 0.12 |
| (1,385) | 1:170:A:PHE:HE2 | 1:222:A:ILE:HD13 | 14 | 0.12 |
| (1,338) | 1:172:A:SER:HA | 1:173:A:TYR:HA | 3 | 0.12 |
| (1,327) | 1:224:A:LEU:H | 1:225:A:LYS:HA | 14 | 0.12 |
| (1,317) | 1:218:A:ALA:HB1 | 1:220:A:LEU:HA | 15 | 0.12 |
| (1,317) | 1:218:A:ALA:HB2 | 1:220:A:LEU:HA | 15 | 0.12 |
| (1,317) | 1:218:A:ALA:HB3 | 1:220:A:LEU:HA | 15 | 0.12 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 5 | 0.12 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 2 | 0.12 |
| (1,303) | 1:70:A:THR:HB | 1:86:A:GLU:HG2 | 15 | 0.12 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 13 | 0.12 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 13 | 0.12 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 13 | 0.12 |
| (1,257) | 1:67:A:ALA:HB1 | 1:90:A:HIS:H | 14 | 0.12 |
| (1,257) | 1:67:A:ALA:HB2 | 1:90:A:HIS:H | 14 | 0.12 |
| (1,257) | 1:67:A:ALA:HB3 | 1:90:A:HIS:H | 14 | 0.12 |
| (1,245) | 1:63:A:TYR:HA | 1:64:A:PRO:HG2 | 5 | 0.12 |
| (1,207) | 1:138:A:ALA:HB1 | 1:139:A:SER:HB2 | 11 | 0.12 |
| (1,207) | 1:138:A:ALA:HB2 | 1:139:A:SER:HB2 | 11 | 0.12 |
| (1,207) | 1:138:A:ALA:HB3 | 1:139:A:SER:HB2 | 11 | 0.12 |
| (1,191) | 1:152:A:LYS:H | 1:168:A:ALA:HA | 1 | 0.12 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 10 | 0.12 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 19 | 0.12 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 19 | 0.12 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 19 | 0.12 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 7 | 0.12 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 7 | 0.12 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 7 | 0.12 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 14 | 0.12 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 14 | 0.12 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 14 | 0.12 |
| (1,152) | 1:212:A:LYS:HB2 | 1:212:A:LYS:HE3 | 18 | 0.12 |
| (1,152) | 1:212:A:LYS:HB3 | 1:212:A:LYS:HE3 | 18 | 0.12 |
| (1,142) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HB3 | 2 | 0.12 |
| (1,142) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HB3 | 2 | 0.12 |
| (1,142) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HB3 | 2 | 0.12 |
| (1,142) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HB3 | 9 | 0.12 |
| (1,142) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HB3 | 9 | 0.12 |
| (1,142) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HB3 | 9 | 0.12 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 8 | 0.12 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 8 | 0.12 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,106) | 1:54:A:ILE:HB | 2:10:B:TYR:H | 20 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 12 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 15 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 19 | 0.12 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 19 | 0.12 |
| (1,80) | 1:53:A:THR:HA | 2:9:B:ILE:HA | 10 | 0.12 |
| (1,79) | 1:70:A:THR:HA | 1:86:A:GLU:HB3 | 13 | 0.12 |
| (1,72) | 1:53:A:THR:HA | 1:54:A:ILE:HG13 | 18 | 0.12 |
| (1,65) | 1:52:A:VAL:HG11 | 1:76:A:MET:H | 4 | 0.12 |
| (1,65) | 1:52:A:VAL:HG12 | 1:76:A:MET:H | 4 | 0.12 |
| (1,65) | 1:52:A:VAL:HG13 | 1:76:A:MET:H | 4 | 0.12 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 17 | 0.12 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 18 | 0.12 |
| (1,51) | 1:122:A:PRO:HD3 | 1:137:A:ASP:HB3 | 16 | 0.12 |
| (1,49) | 1:50:A:LEU:HD21 | 1:51:A:PRO:HD2 | 7 | 0.12 |
| (1,49) | 1:50:A:LEU:HD22 | 1:51:A:PRO:HD2 | 7 | 0.12 |
| (1,49) | 1:50:A:LEU:HD23 | 1:51:A:PRO:HD2 | 7 | 0.12 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 6 | 0.12 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 14 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 17 | 0.12 |
| (1,35) | 1:155:A:LYS:HB3 | 1:155:A:LYS:HE2 | 5 | 0.12 |
| (1,4) | 1:134:A:VAL:HG11 | 1:155:A:LYS:HE2 | 15 | 0.12 |
| (1,4) | 1:134:A:VAL:HG12 | 1:155:A:LYS:HE2 | 15 | 0.12 |
| (1,4) | 1:134:A:VAL:HG13 | 1:155:A:LYS:HE2 | 15 | 0.12 |
| (1,4048) | 2:19:B:GLN:HE21 | 2:21:B:MET:HB3 | 12 | 0.11 |
| (1,4048) | 2:19:B:GLN:HE22 | 2:21:B:MET:HB3 | 12 | 0.11 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB2 | 19 | 0.11 |
| (1,4023) | 2:13:B:ARG:H | 2:14:B:ARG:HB3 | 19 | 0.11 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 17 | 0.11 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 17 | 0.11 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD11 | 2 | 0.11 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD12 | 2 | 0.11 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD13 | 2 | 0.11 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD21 | 2 | 0.11 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD22 | 2 | 0.11 |
| (1,3966) | 1:205:A:LYS:HA | 1:209:A:LEU:HD23 | 2 | 0.11 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB1 | 16 | 0.11 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB2 | 16 | 0.11 |
| (1,3945) | 1:190:A:LYS:HE2 | 1:218:A:ALA:HB3 | 16 | 0.11 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB1 | 16 | 0.11 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB2 | 16 | 0.11 |
| (1,3945) | 1:190:A:LYS:HE3 | 1:218:A:ALA:HB3 | 16 | 0.11 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2 | 18 | 0.11 |
| (1,3915) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3 | 18 | 0.11 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2 | 18 | 0.11 |
| (1,3915) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3 | 18 | 0.11 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2 | 18 | 0.11 |
| (1,3915) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3 | 18 | 0.11 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD11 | 6 | 0.11 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD12 | 6 | 0.11 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD13 | 6 | 0.11 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD21 | 6 | 0.11 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD22 | 6 | 0.11 |
| (1,3910) | 1:181:A:GLU:H | 1:220:A:LEU:HD23 | 6 | 0.11 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD11 | 18 | 0.11 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD12 | 18 | 0.11 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD13 | 18 | 0.11 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD21 | 18 | 0.11 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD22 | 18 | 0.11 |
| (1,3908) | 1:180:A:ILE:HA | 1:209:A:LEU:HD23 | 18 | 0.11 |
| (1,3898) | 1:176:A:ALA:HA | 1:209:A:LEU:HD11 | 14 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3898) | 1:176:A:ALA:HA | 1:209:A:LEU:HD12 | 14 | 0.11 |
| (1,3898) | 1:176:A:ALA:HA | 1:209:A:LEU:HD13 | 14 | 0.11 |
| (1,3898) | 1:176:A:ALA:HA | 1:209:A:LEU:HD21 | 14 | 0.11 |
| (1,3898) | 1:176:A:ALA:HA | 1:209:A:LEU:HD22 | 14 | 0.11 |
| (1,3898) | 1:176:A:ALA:HA | 1:209:A:LEU:HD23 | 14 | 0.11 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB1 | 19 | 0.11 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB2 | 19 | 0.11 |
| (1,3897) | 1:175:A:ASN:HD21 | 1:178:A:ALA:HB3 | 19 | 0.11 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB1 | 19 | 0.11 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB2 | 19 | 0.11 |
| (1,3897) | 1:175:A:ASN:HD22 | 1:178:A:ALA:HB3 | 19 | 0.11 |
| (1,3867) | 1:152:A:LYS:HA | 1:152:A:LYS:HE2 | 2 | 0.11 |
| (1,3867) | 1:152:A:LYS:HA | 1:152:A:LYS:HE3 | 2 | 0.11 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB2 | 2 | 0.11 |
| (1,3859) | 1:149:A:ALA:HA | 1:150:A:SER:HB3 | 2 | 0.11 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 13 | 0.11 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 13 | 0.11 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 20 | 0.11 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 20 | 0.11 |
| (1,3839) | 1:131:A:LYS:HB2 | 1:160:A:GLY:HA3 | 8 | 0.11 |
| (1,3839) | 1:131:A:LYS:HB3 | 1:160:A:GLY:HA3 | 8 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD11 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD12 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD13 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD21 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD22 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD11 | 1:163:A:LEU:HD23 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD11 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD12 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD13 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD21 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD22 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD12 | 1:163:A:LEU:HD23 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD11 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD12 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD13 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD21 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD22 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD13 | 1:163:A:LEU:HD23 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 13 | 0.11 |
| (1,3809) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 13 | 0.11 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG21 | 19 | 0.11 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG22 | 19 | 0.11 |
| (1,3770) | 1:113:A:ASP:HB2 | 1:143:A:VAL:HG23 | 19 | 0.11 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG21 | 19 | 0.11 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG22 | 19 | 0.11 |
| (1,3770) | 1:113:A:ASP:HB3 | 1:143:A:VAL:HG23 | 19 | 0.11 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD11 | 16 | 0.11 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD12 | 16 | 0.11 |
| (1,3769) | 1:113:A:ASP:HB2 | 1:118:A:ILE:HD13 | 16 | 0.11 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD11 | 16 | 0.11 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD12 | 16 | 0.11 |
| (1,3769) | 1:113:A:ASP:HB3 | 1:118:A:ILE:HD13 | 16 | 0.11 |
| (1,3749) | 1:111:A:HIS:HD2 | 1:113:A:ASP:HB2 | 5 | 0.11 |
| (1,3749) | 1:111:A:HIS:HD2 | 1:113:A:ASP:HB3 | 5 | 0.11 |
| (1,3740) | 1:110:A:VAL:HG11 | 1:123:A:LYS:H | 18 | 0.11 |
| (1,3740) | 1:110:A:VAL:HG12 | 1:123:A:LYS:H | 18 | 0.11 |
| (1,3740) | 1:110:A:VAL:HG13 | 1:123:A:LYS:H | 18 | 0.11 |
| (1,3740) | 1:110:A:VAL:HG21 | 1:123:A:LYS:H | 18 | 0.11 |
| (1,3740) | 1:110:A:VAL:HG22 | 1:123:A:LYS:H | 18 | 0.11 |
| (1,3740) | 1:110:A:VAL:HG23 | 1:123:A:LYS:H | 18 | 0.11 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 20 | 0.11 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 20 | 0.11 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 20 | 0.11 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 20 | 0.11 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 20 | 0.11 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 20 | 0.11 |
| (1,3698) | 1:101:A:VAL:HA | 1:102:A:ARG:HB2 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3698) | 1:101:A:VAL:HA | 1:102:A:ARG:HB3 | 6 | 0.11 |
| (1,3691) | 1:97:A:GLN:HB2 | 1:98:A:PRO:HD3 | 6 | 0.11 |
| (1,3691) | 1:97:A:GLN:HB3 | 1:98:A:PRO:HD3 | 6 | 0.11 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB2 | 16 | 0.11 |
| (1,3611) | 1:80:A:SER:HA | 1:114:A:ASP:HB3 | 16 | 0.11 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD2 | 3 | 0.11 |
| (1,3596) | 1:76:A:MET:HG2 | 1:81:A:ARG:HD3 | 3 | 0.11 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD2 | 3 | 0.11 |
| (1,3596) | 1:76:A:MET:HG3 | 1:81:A:ARG:HD3 | 3 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB1 | 1:89:A:LEU:HD11 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB1 | 1:89:A:LEU:HD12 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB1 | 1:89:A:LEU:HD13 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB1 | 1:89:A:LEU:HD21 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB1 | 1:89:A:LEU:HD22 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB1 | 1:89:A:LEU:HD23 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB2 | 1:89:A:LEU:HD11 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB2 | 1:89:A:LEU:HD12 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB2 | 1:89:A:LEU:HD13 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB2 | 1:89:A:LEU:HD21 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB2 | 1:89:A:LEU:HD22 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB2 | 1:89:A:LEU:HD23 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB3 | 1:89:A:LEU:HD11 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB3 | 1:89:A:LEU:HD12 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB3 | 1:89:A:LEU:HD13 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB3 | 1:89:A:LEU:HD21 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB3 | 1:89:A:LEU:HD22 | 10 | 0.11 |
| (1,3581) | 1:67:A:ALA:HB3 | 1:89:A:LEU:HD23 | 10 | 0.11 |
| (1,3507) | 1:52:A:VAL:HB | 2:8:B:ILE:H | 5 | 0.11 |
| (1,3491) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HB3 | 15 | 0.11 |
| (1,3491) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HB3 | 15 | 0.11 |
| (1,3491) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HB3 | 15 | 0.11 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD1 | 12 | 0.11 |
| (1,3487) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HD2 | 12 | 0.11 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD1 | 12 | 0.11 |
| (1,3487) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HD2 | 12 | 0.11 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD1 | 12 | 0.11 |
| (1,3487) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HD2 | 12 | 0.11 |
| (1,3485) | 1:54:A:ILE:HD11 | 2:10:B:TYR:HB2 | 17 | 0.11 |
| (1,3485) | 1:54:A:ILE:HD12 | 2:10:B:TYR:HB2 | 17 | 0.11 |
| (1,3485) | 1:54:A:ILE:HD13 | 2:10:B:TYR:HB2 | 17 | 0.11 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD2 | 15 | 0.11 |
| (1,3464) | 2:9:B:ILE:HG12 | 2:20:B:ARG:HD3 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3451) | 2:6:B:VAL:HG21 | 2:8:B:ILE:H | 1 | 0.11 |
| (1,3451) | 2:6:B:VAL:HG22 | 2:8:B:ILE:H | 1 | 0.11 |
| (1,3451) | 2:6:B:VAL:HG23 | 2:8:B:ILE:H | 1 | 0.11 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD1 | 3 | 0.11 |
| (1,3440) | 2:9:B:ILE:HG21 | 2:10:B:TYR:HD2 | 3 | 0.11 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD1 | 3 | 0.11 |
| (1,3440) | 2:9:B:ILE:HG22 | 2:10:B:TYR:HD2 | 3 | 0.11 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD1 | 3 | 0.11 |
| (1,3440) | 2:9:B:ILE:HG23 | 2:10:B:TYR:HD2 | 3 | 0.11 |
| (1,3405) | 2:8:B:ILE:HD11 | 2:10:B:TYR:HB3 | 4 | 0.11 |
| (1,3405) | 2:8:B:ILE:HD12 | 2:10:B:TYR:HB3 | 4 | 0.11 |
| (1,3405) | 2:8:B:ILE:HD13 | 2:10:B:TYR:HB3 | 4 | 0.11 |
| (1,3345) | 2:15:B:THR:HG21 | 2:17:B:LYS:H | 10 | 0.11 |
| (1,3345) | 2:15:B:THR:HG22 | 2:17:B:LYS:H | 10 | 0.11 |
| (1,3345) | 2:15:B:THR:HG23 | 2:17:B:LYS:H | 10 | 0.11 |
| (1,3278) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HB2 | 3 | 0.11 |
| (1,3278) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HB2 | 3 | 0.11 |
| (1,3272) | 1:111:A:HIS:HB3 | 1:111:A:HIS:HD2 | 7 | 0.11 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB2 | 11 | 0.11 |
| (1,3267) | 1:58:A:HIS:HE1 | 1:60:A:LYS:HB3 | 11 | 0.11 |
| (1,3264) | 1:58:A:HIS:HD2 | 1:60:A:LYS:H | 12 | 0.11 |
| (1,3264) | 1:58:A:HIS:HD2 | 1:60:A:LYS:H | 17 | 0.11 |
| (1,3260) | 1:58:A:HIS:HD2 | 1:70:A:THR:HB | 20 | 0.11 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB1 | 15 | 0.11 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB2 | 15 | 0.11 |
| (1,3244) | 1:182:A:HIS:HD2 | 1:183:A:ALA:HB3 | 15 | 0.11 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 10 | 0.11 |
| (1,3178) | 1:170:A:PHE:HA | 1:170:A:PHE:HD1 | 6 | 0.11 |
| (1,3178) | 1:170:A:PHE:HA | 1:170:A:PHE:HD2 | 6 | 0.11 |
| (1,3178) | 1:170:A:PHE:HA | 1:170:A:PHE:HD1 | 14 | 0.11 |
| (1,3178) | 1:170:A:PHE:HA | 1:170:A:PHE:HD2 | 14 | 0.11 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB1 | 1 | 0.11 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB2 | 1 | 0.11 |
| (1,3131) | 1:63:A:TYR:HD1 | 1:67:A:ALA:HB3 | 1 | 0.11 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB1 | 1 | 0.11 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB2 | 1 | 0.11 |
| (1,3131) | 1:63:A:TYR:HD2 | 1:67:A:ALA:HB3 | 1 | 0.11 |
| (1,3123) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HE1 | 14 | 0.11 |
| (1,3123) | 1:82:A:LEU:HD21 | 1:112:A:TYR:HE2 | 14 | 0.11 |
| (1,3123) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HE1 | 14 | 0.11 |
| (1,3123) | 1:82:A:LEU:HD22 | 1:112:A:TYR:HE2 | 14 | 0.11 |
| (1,3123) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HE1 | 14 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3123) | 1:82:A:LEU:HD23 | 1:112:A:TYR:HE2 | 14 | 0.11 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 9 | 0.11 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 9 | 0.11 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 9 | 0.11 |
| (1,3100) | 1:56:A:ALA:HB1 | 1:73:A:VAL:H | 11 | 0.11 |
| (1,3100) | 1:56:A:ALA:HB2 | 1:73:A:VAL:H | 11 | 0.11 |
| (1,3100) | 1:56:A:ALA:HB3 | 1:73:A:VAL:H | 11 | 0.11 |
| (1,3096) | 1:60:A:LYS:HE3 | 1:61:A:GLY:H | 16 | 0.11 |
| (1,3079) | 1:64:A:PRO:HA | 1:91:A:GLN:HE21 | 17 | 0.11 |
| (1,3069) | 1:195:A:ASN:HB2 | 1:196:A:ASN:HD21 | 8 | 0.11 |
| (1,3049) | 1:196:A:ASN:HB2 | 1:225:A:LYS:H | 1 | 0.11 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 19 | 0.11 |
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 20 | 0.11 |
| (1,3024) | 1:218:A:ALA:HA | 1:219:A:THR:H | 6 | 0.11 |
| (1,3010) | 1:217:A:GLY:H | 1:218:A:ALA:HA | 14 | 0.11 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD21 | 19 | 0.11 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD22 | 19 | 0.11 |
| (1,3002) | 1:215:A:GLU:H | 1:216:A:LEU:HD23 | 19 | 0.11 |
| (1,2978) | 1:201:A:ILE:HD11 | 1:206:A:ALA:H | 20 | 0.11 |
| (1,2978) | 1:201:A:ILE:HD12 | 1:206:A:ALA:H | 20 | 0.11 |
| (1,2978) | 1:201:A:ILE:HD13 | 1:206:A:ALA:H | 20 | 0.11 |
| (1,2951) | 1:198:A:THR:HB | 1:199:A:GLY:H | 10 | 0.11 |
| (1,2923) | 1:194:A:ILE:HG12 | 1:195:A:ASN:H | 9 | 0.11 |
| (1,2882) | 1:187:A:MET:H | 1:187:A:MET:HG2 | 8 | 0.11 |
| (1,2856) | 1:142:A:THR:HG21 | 1:182:A:HIS:H | 5 | 0.11 |
| (1,2856) | 1:142:A:THR:HG22 | 1:182:A:HIS:H | 5 | 0.11 |
| (1,2856) | 1:142:A:THR:HG23 | 1:182:A:HIS:H | 5 | 0.11 |
| (1,2818) | 1:175:A:ASN:HB3 | 1:176:A:ALA:H | 8 | 0.11 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 10 | 0.11 |
| (1,2810) | 1:174:A:GLU:HG3 | 1:175:A:ASN:H | 18 | 0.11 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB1 | 12 | 0.11 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB2 | 12 | 0.11 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB3 | 12 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE1 | 7 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE2 | 7 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE1 | 8 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE2 | 8 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE1 | 17 | 0.11 |
| (1,2775) | 1:170:A:PHE:H | 1:170:A:PHE:HE2 | 17 | 0.11 |
| (1,2752) | 1:154:A:ILE:HA | 1:166:A:ASP:H | 3 | 0.11 |
| (1,2752) | 1:154:A:ILE:HA | 1:166:A:ASP:H | 9 | 0.11 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD11 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD12 | 15 | 0.11 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD13 | 15 | 0.11 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD21 | 15 | 0.11 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD22 | 15 | 0.11 |
| (1,2714) | 1:157:A:LEU:H | 1:163:A:LEU:HD23 | 15 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD21 | 11 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD22 | 11 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD23 | 11 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD21 | 13 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD22 | 13 | 0.11 |
| (1,2713) | 1:157:A:LEU:H | 1:157:A:LEU:HD23 | 13 | 0.11 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 2 | 0.11 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 5 | 0.11 |
| (1,2667) | 1:139:A:SER:HA | 1:151:A:ALA:H | 10 | 0.11 |
| (1,2649) | 1:141:A:GLU:HA | 1:149:A:ALA:H | 14 | 0.11 |
| (1,2625) | 1:143:A:VAL:H | 1:145:A:ALA:H | 20 | 0.11 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB1 | 9 | 0.11 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB2 | 9 | 0.11 |
| (1,2609) | 1:142:A:THR:H | 1:145:A:ALA:HB3 | 9 | 0.11 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 20 | 0.11 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 8 | 0.11 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 20 | 0.11 |
| (1,2574) | 1:136:A:TYR:HB3 | 1:138:A:ALA:H | 10 | 0.11 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 20 | 0.11 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 20 | 0.11 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 20 | 0.11 |
| (1,2543) | 1:130:A:THR:HG21 | 1:131:A:LYS:H | 4 | 0.11 |
| (1,2543) | 1:130:A:THR:HG22 | 1:131:A:LYS:H | 4 | 0.11 |
| (1,2543) | 1:130:A:THR:HG23 | 1:131:A:LYS:H | 4 | 0.11 |
| (1,2473) | 1:118:A:ILE:H | 1:119:A:LEU:HD11 | 14 | 0.11 |
| (1,2473) | 1:118:A:ILE:H | 1:119:A:LEU:HD12 | 14 | 0.11 |
| (1,2473) | 1:118:A:ILE:H | 1:119:A:LEU:HD13 | 14 | 0.11 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 1 | 0.11 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 1 | 0.11 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 6 | 0.11 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 6 | 0.11 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 19 | 0.11 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 19 | 0.11 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 2 | 0.11 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 14 | 0.11 |
| (1,2413) | 1:108:A:GLY:H | 1:109:A:ASN:H | 4 | 0.11 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG11 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG12 | 3 | 0.11 |
| (1,2390) | 1:103:A:THR:H | 1:104:A:VAL:HG13 | 3 | 0.11 |
| (1,2354) | 1:87:A:VAL:HB | 1:88:A:GLN:H | 13 | 0.11 |
| (1,2314) | 1:83:A:GLN:H | 1:83:A:GLN:HB3 | 17 | 0.11 |
| (1,2314) | 1:83:A:GLN:H | 1:83:A:GLN:HB3 | 20 | 0.11 |
| (1,2311) | 1:82:A:LEU:H | 1:112:A:TYR:HD1 | 1 | 0.11 |
| (1,2311) | 1:82:A:LEU:H | 1:112:A:TYR:HD2 | 1 | 0.11 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 2 | 0.11 |
| (1,2306) | 1:82:A:LEU:H | 1:82:A:LEU:HB3 | 3 | 0.11 |
| (1,2302) | 1:77:A:GLN:HB3 | 1:80:A:SER:H | 17 | 0.11 |
| (1,2291) | 1:75:A:ILE:HG12 | 1:76:A:MET:H | 5 | 0.11 |
| (1,2279) | 1:75:A:ILE:H | 1:84:A:ALA:H | 13 | 0.11 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 14 | 0.11 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 18 | 0.11 |
| (1,2110) | 1:56:A:ALA:HB1 | 1:73:A:VAL:HB | 7 | 0.11 |
| (1,2110) | 1:56:A:ALA:HB2 | 1:73:A:VAL:HB | 7 | 0.11 |
| (1,2110) | 1:56:A:ALA:HB3 | 1:73:A:VAL:HB | 7 | 0.11 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG21 | 3 | 0.11 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG22 | 3 | 0.11 |
| (1,2108) | 1:51:A:PRO:HB3 | 2:6:B:VAL:HG23 | 3 | 0.11 |
| (1,2104) | 1:47:A:THR:HB | 1:48:A:ASN:HB3 | 3 | 0.11 |
| (1,2096) | 1:47:A:THR:HA | 1:50:A:LEU:HG | 16 | 0.11 |
| (1,2083) | 1:223:A:THR:HB | 1:224:A:LEU:HB2 | 14 | 0.11 |
| (1,2083) | 1:223:A:THR:HB | 1:224:A:LEU:HB3 | 14 | 0.11 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG21 | 5 | 0.11 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG22 | 5 | 0.11 |
| (1,2065) | 1:207:A:THR:H | 1:222:A:ILE:HG23 | 5 | 0.11 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 2 | 0.11 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 2 | 0.11 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 2 | 0.11 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 13 | 0.11 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 13 | 0.11 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 13 | 0.11 |
| (1,2041) | 1:157:A:LEU:HD21 | 1:162:A:THR:HB | 1 | 0.11 |
| (1,2041) | 1:157:A:LEU:HD22 | 1:162:A:THR:HB | 1 | 0.11 |
| (1,2041) | 1:157:A:LEU:HD23 | 1:162:A:THR:HB | 1 | 0.11 |
| (1,2039) | 1:54:A:ILE:HG12 | 2:10:B:TYR:HB2 | 4 | 0.11 |
| (1,2018) | 1:218:A:ALA:HA | 1:219:A:THR:HA | 14 | 0.11 |
| (1,1963) | 1:161:A:LYS:HD2 | 1:189:A:VAL:H | 5 | 0.11 |
| (1,1963) | 1:161:A:LYS:HD3 | 1:189:A:VAL:H | 5 | 0.11 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 2 | 0.11 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 2 | 0.11 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 2 | 0.11 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 2 | 0.11 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 2 | 0.11 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 8 | 0.11 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 8 | 0.11 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 16 | 0.11 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 16 | 0.11 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 19 | 0.11 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 19 | 0.11 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB2 | 11 | 0.11 |
| (1,1888) | 1:207:A:THR:HB | 1:208:A:LYS:HB3 | 11 | 0.11 |
| (1,1856) | 1:202:A:THR:H | 1:205:A:LYS:HA | 8 | 0.11 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB1 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB2 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB3 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB1 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB2 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB3 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB1 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB2 | 5 | 0.11 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB3 | 5 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 2 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 2 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 2 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 6 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 6 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 6 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 13 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 13 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 13 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 14 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 14 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 14 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 16 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 16 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 16 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB1 | 1:222:A:ILE:HA | 19 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB2 | 1:222:A:ILE:HA | 19 | 0.11 |
| (1,1844) | 1:206:A:ALA:HB3 | 1:222:A:ILE:HA | 19 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG21 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG22 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1823) | 1:194:A:ILE:HG21 | 1:201:A:ILE:HG23 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG21 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG22 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG22 | 1:201:A:ILE:HG23 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG21 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG22 | 15 | 0.11 |
| (1,1823) | 1:194:A:ILE:HG23 | 1:201:A:ILE:HG23 | 15 | 0.11 |
| (1,1815) | 1:201:A:ILE:HG21 | 1:205:A:LYS:H | 17 | 0.11 |
| (1,1815) | 1:201:A:ILE:HG22 | 1:205:A:LYS:H | 17 | 0.11 |
| (1,1815) | 1:201:A:ILE:HG23 | 1:205:A:LYS:H | 17 | 0.11 |
| (1,1795) | 1:201:A:ILE:HD11 | 1:202:A:THR:H | 2 | 0.11 |
| (1,1795) | 1:201:A:ILE:HD12 | 1:202:A:THR:H | 2 | 0.11 |
| (1,1795) | 1:201:A:ILE:HD13 | 1:202:A:THR:H | 2 | 0.11 |
| (1,1795) | 1:201:A:ILE:HD11 | 1:202:A:THR:H | 18 | 0.11 |
| (1,1795) | 1:201:A:ILE:HD12 | 1:202:A:THR:H | 18 | 0.11 |
| (1,1795) | 1:201:A:ILE:HD13 | 1:202:A:THR:H | 18 | 0.11 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 4 | 0.11 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 4 | 0.11 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 4 | 0.11 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD11 | 11 | 0.11 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD12 | 11 | 0.11 |
| (1,1789) | 1:171:A:ASP:H | 1:201:A:ILE:HD13 | 11 | 0.11 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 6 | 0.11 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 6 | 0.11 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 6 | 0.11 |
| (1,1764) | 1:169:A:THR:HG21 | 1:199:A:GLY:HA3 | 19 | 0.11 |
| (1,1764) | 1:169:A:THR:HG22 | 1:199:A:GLY:HA3 | 19 | 0.11 |
| (1,1764) | 1:169:A:THR:HG23 | 1:199:A:GLY:HA3 | 19 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB1 | 1:201:A:ILE:HD11 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB1 | 1:201:A:ILE:HD12 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB1 | 1:201:A:ILE:HD13 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB2 | 1:201:A:ILE:HD11 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB2 | 1:201:A:ILE:HD12 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB2 | 1:201:A:ILE:HD13 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB3 | 1:201:A:ILE:HD11 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB3 | 1:201:A:ILE:HD12 | 3 | 0.11 |
| (1,1754) | 1:197:A:ALA:HB3 | 1:201:A:ILE:HD13 | 3 | 0.11 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB1 | 6 | 0.11 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB2 | 6 | 0.11 |
| (1,1749) | 1:170:A:PHE:HB2 | 1:197:A:ALA:HB3 | 6 | 0.11 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 15 | 0.11 |
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1730) | 1:195:A:ASN:HA | 1:196:A:ASN:HB3 | 20 | 0.11 |
| (1,1724) | 1:167:A:ASP:HA | 1:196:A:ASN:HA | 4 | 0.11 |
| (1,1716) | 1:195:A:ASN:HA | 1:223:A:THR:HB | 9 | 0.11 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD11 | 10 | 0.11 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD12 | 10 | 0.11 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD13 | 10 | 0.11 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD11 | 12 | 0.11 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD12 | 12 | 0.11 |
| (1,1699) | 1:165:A:PHE:HB3 | 1:194:A:ILE:HD13 | 12 | 0.11 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD11 | 6 | 0.11 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD12 | 6 | 0.11 |
| (1,1694) | 1:192:A:ILE:HA | 1:194:A:ILE:HD13 | 6 | 0.11 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD11 | 15 | 0.11 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD12 | 15 | 0.11 |
| (1,1692) | 1:180:A:ILE:H | 1:194:A:ILE:HD13 | 15 | 0.11 |
| (1,1691) | 1:194:A:ILE:HD11 | 1:223:A:THR:H | 5 | 0.11 |
| (1,1691) | 1:194:A:ILE:HD12 | 1:223:A:THR:H | 5 | 0.11 |
| (1,1691) | 1:194:A:ILE:HD13 | 1:223:A:THR:H | 5 | 0.11 |
| (1,1674) | 1:192:A:ILE:HG21 | 1:193:A:THR:HB | 1 | 0.11 |
| (1,1674) | 1:192:A:ILE:HG22 | 1:193:A:THR:HB | 1 | 0.11 |
| (1,1674) | 1:192:A:ILE:HG23 | 1:193:A:THR:HB | 1 | 0.11 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 19 | 0.11 |
| (1,1632) | 1:190:A:LYS:HB3 | 1:191:A:THR:HA | 11 | 0.11 |
| (1,1622) | 1:162:A:THR:HG21 | 1:191:A:THR:H | 8 | 0.11 |
| (1,1622) | 1:162:A:THR:HG22 | 1:191:A:THR:H | 8 | 0.11 |
| (1,1622) | 1:162:A:THR:HG23 | 1:191:A:THR:H | 8 | 0.11 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 7 | 0.11 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 7 | 0.11 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 7 | 0.11 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 7 | 0.11 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 8 | 0.11 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 8 | 0.11 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE2 | 16 | 0.11 |
| (1,1590) | 1:225:A:LYS:H | 1:225:A:LYS:HE3 | 16 | 0.11 |
| (1,1545) | 1:184:A:ILE:HA | 1:189:A:VAL:HA | 19 | 0.11 |
| (1,1534) | 1:183:A:ALA:HB1 | 1:184:A:ILE:HG13 | 3 | 0.11 |
| (1,1534) | 1:183:A:ALA:HB2 | 1:184:A:ILE:HG13 | 3 | 0.11 |
| (1,1534) | 1:183:A:ALA:HB3 | 1:184:A:ILE:HG13 | 3 | 0.11 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 3 | 0.11 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 3 | 0.11 |
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 7 | 0.11 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1511) | 1:181:A:GLU:HB2 | 1:182:A:HIS:HB3 | 12 | 0.11 |
| (1,1511) | 1:181:A:GLU:HB3 | 1:182:A:HIS:HB3 | 12 | 0.11 |
| (1,1505) | 1:180:A:ILE:HG13 | 1:181:A:GLU:HA | 5 | 0.11 |
| (1,1501) | 1:180:A:ILE:HG21 | 1:192:A:ILE:H | 7 | 0.11 |
| (1,1501) | 1:180:A:ILE:HG22 | 1:192:A:ILE:H | 7 | 0.11 |
| (1,1501) | 1:180:A:ILE:HG23 | 1:192:A:ILE:H | 7 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 5 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 5 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 5 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 6 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 6 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 6 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 10 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 10 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 10 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG21 | 1:209:A:LEU:HA | 20 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG22 | 1:209:A:LEU:HA | 20 | 0.11 |
| (1,1498) | 1:180:A:ILE:HG23 | 1:209:A:LEU:HA | 20 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 5 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 5 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 5 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 6 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 6 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 6 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 7 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 7 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 7 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 8 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 8 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 8 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 10 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 10 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 10 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 11 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 11 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 11 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 12 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 12 | 0.11 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 12 | 0.11 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD11 | 10 | 0.11 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD12 | 10 | 0.11 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD13 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD21 | 10 | 0.11 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD22 | 10 | 0.11 |
| (1,1478) | 1:147:A:GLY:HA3 | 1:179:A:LEU:HD23 | 10 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB1 | 11 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB2 | 11 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB3 | 11 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB1 | 17 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB2 | 17 | 0.11 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB3 | 17 | 0.11 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 4 | 0.11 |
| (1,1451) | 1:175:A:ASN:HA | 1:178:A:ALA:HA | 9 | 0.11 |
| (1,1447) | 1:178:A:ALA:HA | 1:182:A:HIS:HB3 | 3 | 0.11 |
| (1,1441) | 1:142:A:THR:HG21 | 1:178:A:ALA:HA | 5 | 0.11 |
| (1,1441) | 1:142:A:THR:HG22 | 1:178:A:ALA:HA | 5 | 0.11 |
| (1,1441) | 1:142:A:THR:HG23 | 1:178:A:ALA:HA | 5 | 0.11 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 16 | 0.11 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 16 | 0.11 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 16 | 0.11 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB1 | 20 | 0.11 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB2 | 20 | 0.11 |
| (1,1429) | 1:170:A:PHE:HB2 | 1:176:A:ALA:HB3 | 20 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 2 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 3 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 5 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 6 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 8 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 9 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 10 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 13 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 14 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 15 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 18 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 19 | 0.11 |
| (1,1408) | 1:174:A:GLU:HB2 | 1:174:A:GLU:HG3 | 20 | 0.11 |
| (1,1401) | 1:172:A:SER:HA | 1:174:A:GLU:HB2 | 8 | 0.11 |
| (1,1367) | 1:167:A:ASP:HA | 1:195:A:ASN:H | 8 | 0.11 |
| (1,1359) | 1:166:A:ASP:HA | 1:195:A:ASN:HD22 | 8 | 0.11 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB1 | 18 | 0.11 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB2 | 18 | 0.11 |
| (1,1356) | 1:166:A:ASP:HA | 1:168:A:ALA:HB3 | 18 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 2 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 8 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 8 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 10 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 10 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 11 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 11 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 15 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 15 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 18 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 18 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 20 | 0.11 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 20 | 0.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG21 | 5 | 0.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG22 | 5 | 0.11 |
| (1,1332) | 1:156:A:SER:HA | 1:162:A:THR:HG23 | 5 | 0.11 |
| (1,1310) | 1:161:A:LYS:HG3 | 1:189:A:VAL:HA | 13 | 0.11 |
| (1,1269) | 1:156:A:SER:HA | 1:157:A:LEU:HB3 | 10 | 0.11 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 14 | 0.11 |
| (1,1192) | 1:136:A:TYR:HA | 1:152:A:LYS:HA | 1 | 0.11 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB1 | 6 | 0.11 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB2 | 6 | 0.11 |
| (1,1171) | 1:151:A:ALA:HA | 1:168:A:ALA:HB3 | 6 | 0.11 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD1 | 13 | 0.11 |
| (1,1170) | 1:80:A:SER:HB3 | 1:112:A:TYR:HD2 | 13 | 0.11 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 4 | 0.11 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 4 | 0.11 |
| (1,1158) | 1:148:A:SER:HB2 | 1:178:A:ALA:HB1 | 3 | 0.11 |
| (1,1158) | 1:148:A:SER:HB2 | 1:178:A:ALA:HB2 | 3 | 0.11 |
| (1,1158) | 1:148:A:SER:HB2 | 1:178:A:ALA:HB3 | 3 | 0.11 |
| (1,1158) | 1:148:A:SER:HB3 | 1:178:A:ALA:HB1 | 3 | 0.11 |
| (1,1158) | 1:148:A:SER:HB3 | 1:178:A:ALA:HB2 | 3 | 0.11 |
| (1,1158) | 1:148:A:SER:HB3 | 1:178:A:ALA:HB3 | 3 | 0.11 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 4 | 0.11 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 9 | 0.11 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 5 | 0.11 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 5 | 0.11 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 5 | 0.11 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB1 | 14 | 0.11 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB2 | 14 | 0.11 |
| (1,1142) | 1:146:A:PRO:HB2 | 1:178:A:ALA:HB3 | 14 | 0.11 |
| (1,1127) | 1:117:A:VAL:HA | 1:143:A:VAL:HA | 12 | 0.11 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 20 | 0.11 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 20 | 0.11 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 20 | 0.11 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 20 | 0.11 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 20 | 0.11 |
| (1,1047) | 1:120:A:LYS:HB2 | 1:139:A:SER:HB2 | 2 | 0.11 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 7 | 0.11 |
| (1,1034) | 1:120:A:LYS:H | 1:138:A:ALA:HA | 12 | 0.11 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 1 | 0.11 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 11 | 0.11 |
| (1,1012) | 1:137:A:ASP:HA | 1:153:A:VAL:H | 13 | 0.11 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 11 | 0.11 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 18 | 0.11 |
| (1,997) | 1:136:A:TYR:HA | 1:154:A:ILE:HG13 | 20 | 0.11 |
| (1,990) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HB | 9 | 0.11 |
| (1,966) | 1:134:A:VAL:HA | 1:155:A:LYS:HG3 | 7 | 0.11 |
| (1,966) | 1:134:A:VAL:HA | 1:155:A:LYS:HG3 | 10 | 0.11 |
| (1,950) | 1:130:A:THR:HB | 1:131:A:LYS:H | 20 | 0.11 |
| (1,942) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HD11 | 17 | 0.11 |
| (1,942) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HD12 | 17 | 0.11 |
| (1,942) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HD13 | 17 | 0.11 |
| (1,942) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HD21 | 17 | 0.11 |
| (1,942) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HD22 | 17 | 0.11 |
| (1,942) | 1:77:A:GLN:HE21 | 1:128:A:LEU:HD23 | 17 | 0.11 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 20 | 0.11 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 20 | 0.11 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 20 | 0.11 |
| (1,846) | 1:162:A:THR:HG21 | 1:163:A:LEU:HA | 17 | 0.11 |
| (1,846) | 1:162:A:THR:HG22 | 1:163:A:LEU:HA | 17 | 0.11 |
| (1,846) | 1:162:A:THR:HG23 | 1:163:A:LEU:HA | 17 | 0.11 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 3 | 0.11 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 3 | 0.11 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 3 | 0.11 |
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 9 | 0.11 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 9 | 0.11 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 9 | 0.11 |
| (1,789) | 1:115:A:ASN:HB2 | 1:116:A:GLN:HA | 12 | 0.11 |
| (1,789) | 1:115:A:ASN:HB3 | 1:116:A:GLN:HA | 12 | 0.11 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG21 | 13 | 0.11 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG22 | 13 | 0.11 |
| (1,783) | 1:115:A:ASN:HA | 1:143:A:VAL:HG23 | 13 | 0.11 |
| (1,776) | 1:113:A:ASP:HA | 1:118:A:ILE:HG12 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,769) | 1:82:A:LEU:HG | 1:112:A:TYR:HA | 6 | 0.11 |
| (1,769) | 1:82:A:LEU:HG | 1:112:A:TYR:HA | 7 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 6 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 6 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 6 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 6 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 6 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 6 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD11 | 19 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD12 | 19 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD13 | 19 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD21 | 19 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD22 | 19 | 0.11 |
| (1,721) | 1:105:A:ASP:H | 1:107:A:LEU:HD23 | 19 | 0.11 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB2 | 13 | 0.11 |
| (1,713) | 1:87:A:VAL:HA | 1:107:A:LEU:HB3 | 13 | 0.11 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 17 | 0.11 |
| (1,664) | 1:103:A:THR:HA | 1:128:A:LEU:H | 18 | 0.11 |
| (1,655) | 1:102:A:ARG:HD2 | 1:103:A:THR:H | 16 | 0.11 |
| (1,655) | 1:102:A:ARG:HD3 | 1:103:A:THR:H | 16 | 0.11 |
| (1,638) | 1:100:A:PRO:HG3 | 1:101:A:VAL:H | 7 | 0.11 |
| (1,630) | 1:98:A:PRO:HA | 1:99:A:GLU:HG2 | 8 | 0.11 |
| (1,630) | 1:98:A:PRO:HA | 1:99:A:GLU:HG3 | 8 | 0.11 |
| (1,629) | 1:99:A:GLU:HG2 | 1:100:A:PRO:HD3 | 10 | 0.11 |
| (1,629) | 1:99:A:GLU:HG3 | 1:100:A:PRO:HD3 | 10 | 0.11 |
| (1,619) | 1:98:A:PRO:HB2 | 1:99:A:GLU:HA | 6 | 0.11 |
| (1,619) | 1:98:A:PRO:HB2 | 1:99:A:GLU:HA | 13 | 0.11 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 10 | 0.11 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 10 | 0.11 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 17 | 0.11 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 17 | 0.11 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 18 | 0.11 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 18 | 0.11 |
| (1,607) | 1:215:A:GLU:HB2 | 1:216:A:LEU:HA | 20 | 0.11 |
| (1,607) | 1:215:A:GLU:HB3 | 1:216:A:LEU:HA | 20 | 0.11 |
| (1,600) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HG3 | 8 | 0.11 |
| (1,600) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HG3 | 8 | 0.11 |
| (1,600) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HG3 | 8 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 2 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 2 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 2 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 2 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 2 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 7 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 7 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 7 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 7 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 7 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 7 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD21 | 14 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD22 | 14 | 0.11 |
| (1,587) | 1:212:A:LYS:HG2 | 1:216:A:LEU:HD23 | 14 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD21 | 14 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD22 | 14 | 0.11 |
| (1,587) | 1:212:A:LYS:HG3 | 1:216:A:LEU:HD23 | 14 | 0.11 |
| (1,547) | 1:107:A:LEU:HA | 1:107:A:LEU:HG | 10 | 0.11 |
| (1,526) | 1:87:A:VAL:HG11 | 1:104:A:VAL:HA | 18 | 0.11 |
| (1,526) | 1:87:A:VAL:HG12 | 1:104:A:VAL:HA | 18 | 0.11 |
| (1,526) | 1:87:A:VAL:HG13 | 1:104:A:VAL:HA | 18 | 0.11 |
| (1,526) | 1:87:A:VAL:HG21 | 1:104:A:VAL:HA | 18 | 0.11 |
| (1,526) | 1:87:A:VAL:HG22 | 1:104:A:VAL:HA | 18 | 0.11 |
| (1,526) | 1:87:A:VAL:HG23 | 1:104:A:VAL:HA | 18 | 0.11 |
| (1,518) | 1:71:A:GLY:H | 1:86:A:GLU:HG3 | 2 | 0.11 |
| (1,444) | 1:77:A:GLN:HA | 1:78:A:GLY:HA3 | 8 | 0.11 |
| (1,442) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HG3 | 8 | 0.11 |
| (1,442) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HG3 | 8 | 0.11 |
| (1,442) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HG3 | 8 | 0.11 |
| (1,412) | 1:75:A:ILE:HG21 | 1:83:A:GLN:HA | 19 | 0.11 |
| (1,412) | 1:75:A:ILE:HG22 | 1:83:A:GLN:HA | 19 | 0.11 |
| (1,412) | 1:75:A:ILE:HG23 | 1:83:A:GLN:HA | 19 | 0.11 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD11 | 17 | 0.11 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD12 | 17 | 0.11 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD13 | 17 | 0.11 |
| (1,338) | 1:172:A:SER:HA | 1:173:A:TYR:HA | 15 | 0.11 |
| (1,320) | 1:58:A:HIS:HB3 | 1:71:A:GLY:HA3 | 2 | 0.11 |
| (1,320) | 1:58:A:HIS:HB3 | 1:71:A:GLY:HA3 | 14 | 0.11 |
| (1,317) | 1:218:A:ALA:HB1 | 1:220:A:LEU:HA | 17 | 0.11 |
| (1,317) | 1:218:A:ALA:HB2 | 1:220:A:LEU:HA | 17 | 0.11 |
| (1,317) | 1:218:A:ALA:HB3 | 1:220:A:LEU:HA | 17 | 0.11 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 3 | 0.11 |
| (1,308) | 1:70:A:THR:HB | 1:87:A:VAL:H | 13 | 0.11 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG21 | 2 | 0.11 |
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG22 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,302) | 1:70:A:THR:HB | 1:73:A:VAL:HG23 | 2 | 0.11 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 16 | 0.11 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 16 | 0.11 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 16 | 0.11 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 20 | 0.11 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 20 | 0.11 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 20 | 0.11 |
| (1,242) | 1:142:A:THR:HG21 | 1:146:A:PRO:HD2 | 7 | 0.11 |
| (1,242) | 1:142:A:THR:HG22 | 1:146:A:PRO:HD2 | 7 | 0.11 |
| (1,242) | 1:142:A:THR:HG23 | 1:146:A:PRO:HD2 | 7 | 0.11 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB1 | 7 | 0.11 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB2 | 7 | 0.11 |
| (1,177) | 1:58:A:HIS:HB2 | 1:59:A:ALA:HB3 | 7 | 0.11 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 1 | 0.11 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 1 | 0.11 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 1 | 0.11 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 2 | 0.11 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 2 | 0.11 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 2 | 0.11 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 7 | 0.11 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 7 | 0.11 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 7 | 0.11 |
| (1,164) | 1:56:A:ALA:HB1 | 1:58:A:HIS:HB3 | 15 | 0.11 |
| (1,164) | 1:56:A:ALA:HB2 | 1:58:A:HIS:HB3 | 15 | 0.11 |
| (1,164) | 1:56:A:ALA:HB3 | 1:58:A:HIS:HB3 | 15 | 0.11 |
| (1,142) | 1:54:A:ILE:HG21 | 1:55:A:ASN:HB3 | 16 | 0.11 |
| (1,142) | 1:54:A:ILE:HG22 | 1:55:A:ASN:HB3 | 16 | 0.11 |
| (1,142) | 1:54:A:ILE:HG23 | 1:55:A:ASN:HB3 | 16 | 0.11 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE1 | 15 | 0.11 |
| (1,138) | 1:55:A:ASN:HA | 2:10:B:TYR:HE2 | 15 | 0.11 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG21 | 12 | 0.11 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG22 | 12 | 0.11 |
| (1,136) | 1:55:A:ASN:HA | 2:9:B:ILE:HG23 | 12 | 0.11 |
| (1,119) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HD11 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HD12 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG11 | 1:54:A:ILE:HD13 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HD11 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HD12 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG12 | 1:54:A:ILE:HD13 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HD11 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HD12 | 3 | 0.11 |
| (1,119) | 1:52:A:VAL:HG13 | 1:54:A:ILE:HD13 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 2 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 4 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 11 | 0.11 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 11 | 0.11 |
| (1,87) | 1:53:A:THR:HB | 1:55:A:ASN:HD22 | 8 | 0.11 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 11 | 0.11 |
| (1,79) | 1:70:A:THR:HA | 1:86:A:GLU:HB3 | 7 | 0.11 |
| (1,69) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE21 | 4 | 0.11 |
| (1,69) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE21 | 4 | 0.11 |
| (1,69) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE21 | 4 | 0.11 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 3 | 0.11 |
| (1,60) | 1:98:A:PRO:HB3 | 1:99:A:GLU:H | 19 | 0.11 |
| (1,55) | 1:50:A:LEU:H | 1:51:A:PRO:HD3 | 13 | 0.11 |
| (1,51) | 1:122:A:PRO:HD3 | 1:137:A:ASP:HB3 | 3 | 0.11 |
| (1,42) | 1:210:A:LYS:HB2 | 1:211:A:ALA:H | 2 | 0.11 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG21 | 2 | 0.11 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG22 | 2 | 0.11 |
| (1,38) | 1:51:A:PRO:HB2 | 2:6:B:VAL:HG23 | 2 | 0.11 |
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG2 | 11 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4012) | 2:10:B:TYR:HB3 | 2:21:B:MET:HG3 | 11 | 0.1 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB2 | 19 | 0.1 |
| (1,4004) | 2:9:B:ILE:HG21 | 2:11:B:CYS:HB3 | 19 | 0.1 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB2 | 19 | 0.1 |
| (1,4004) | 2:9:B:ILE:HG22 | 2:11:B:CYS:HB3 | 19 | 0.1 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB2 | 19 | 0.1 |
| (1,4004) | 2:9:B:ILE:HG23 | 2:11:B:CYS:HB3 | 19 | 0.1 |
| (1,4000) | 2:5:B:PRO:HB2 | 2:6:B:VAL:H | 14 | 0.1 |
| (1,4000) | 2:5:B:PRO:HB3 | 2:6:B:VAL:H | 14 | 0.1 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD21 | 6 | 0.1 |
| (1,3857) | 1:147:A:GLY:HA2 | 1:175:A:ASN:HD22 | 6 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 12 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 12 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 12 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 12 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 12 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 12 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 14 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 14 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 14 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 14 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 14 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 14 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG11 | 1:121:A:GLY:H | 16 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG12 | 1:121:A:GLY:H | 16 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG13 | 1:121:A:GLY:H | 16 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 16 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 16 | 0.1 |
| (1,3738) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 16 | 0.1 |
| (1,3704) | 1:102:A:ARG:HA | 1:102:A:ARG:HG2 | 10 | 0.1 |
| (1,3704) | 1:102:A:ARG:HA | 1:102:A:ARG:HG3 | 10 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE21 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG11 | 1:88:A:GLN:HE22 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE21 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG12 | 1:88:A:GLN:HE22 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE21 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG13 | 1:88:A:GLN:HE22 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE21 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG21 | 1:88:A:GLN:HE22 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE21 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG22 | 1:88:A:GLN:HE22 | 12 | 0.1 |
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE21 | 12 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3647) | 1:87:A:VAL:HG23 | 1:88:A:GLN:HE22 | 12 | 0.1 |
| (1,3613) | 1:80:A:SER:HB2 | 1:81:A:ARG:HA | 9 | 0.1 |
| (1,3613) | 1:80:A:SER:HB3 | 1:81:A:ARG:HA | 9 | 0.1 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA2 | 3 | 0.1 |
| (1,3601) | 1:77:A:GLN:HB3 | 1:78:A:GLY:HA3 | 3 | 0.1 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD21 | 18 | 0.1 |
| (1,3534) | 1:47:A:THR:HA | 1:48:A:ASN:HD22 | 18 | 0.1 |
| (1,3521) | 1:59:A:ALA:HB1 | 2:12:B:ASN:HB2 | 13 | 0.1 |
| (1,3521) | 1:59:A:ALA:HB2 | 2:12:B:ASN:HB2 | 13 | 0.1 |
| (1,3521) | 1:59:A:ALA:HB3 | 2:12:B:ASN:HB2 | 13 | 0.1 |
| (1,3493) | 1:54:A:ILE:HG21 | 2:10:B:TYR:HA | 19 | 0.1 |
| (1,3493) | 1:54:A:ILE:HG22 | 2:10:B:TYR:HA | 19 | 0.1 |
| (1,3493) | 1:54:A:ILE:HG23 | 2:10:B:TYR:HA | 19 | 0.1 |
| (1,3481) | 1:53:A:THR:HG21 | 2:11:B:CYS:HB3 | 14 | 0.1 |
| (1,3481) | 1:53:A:THR:HG22 | 2:11:B:CYS:HB3 | 14 | 0.1 |
| (1,3481) | 1:53:A:THR:HG23 | 2:11:B:CYS:HB3 | 14 | 0.1 |
| (1,3479) | 1:53:A:THR:HG21 | 2:9:B:ILE:HB | 18 | 0.1 |
| (1,3479) | 1:53:A:THR:HG22 | 2:9:B:ILE:HB | 18 | 0.1 |
| (1,3479) | 1:53:A:THR:HG23 | 2:9:B:ILE:HB | 18 | 0.1 |
| (1,3411) | 2:8:B:ILE:HD11 | 2:21:B:MET:HB2 | 15 | 0.1 |
| (1,3411) | 2:8:B:ILE:HD12 | 2:21:B:MET:HB2 | 15 | 0.1 |
| (1,3411) | 2:8:B:ILE:HD13 | 2:21:B:MET:HB2 | 15 | 0.1 |
| (1,3277) | 1:69:A:PHE:HD1 | 1:87:A:VAL:HB | 18 | 0.1 |
| (1,3277) | 1:69:A:PHE:HD2 | 1:87:A:VAL:HB | 18 | 0.1 |
| (1,3272) | 1:111:A:HIS:HB3 | 1:111:A:HIS:HD2 | 10 | 0.1 |
| (1,3246) | 1:142:A:THR:HG21 | 1:182:A:HIS:HD2 | 3 | 0.1 |
| (1,3246) | 1:142:A:THR:HG22 | 1:182:A:HIS:HD2 | 3 | 0.1 |
| (1,3246) | 1:142:A:THR:HG23 | 1:182:A:HIS:HD2 | 3 | 0.1 |
| (1,3210) | 1:133:A:TRP:HH2 | 1:165:A:PHE:HZ | 18 | 0.1 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD1 | 8 | 0.1 |
| (1,3168) | 1:119:A:LEU:HD21 | 1:135:A:PHE:HD2 | 8 | 0.1 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD1 | 8 | 0.1 |
| (1,3168) | 1:119:A:LEU:HD22 | 1:135:A:PHE:HD2 | 8 | 0.1 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD1 | 8 | 0.1 |
| (1,3168) | 1:119:A:LEU:HD23 | 1:135:A:PHE:HD2 | 8 | 0.1 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE1 | 7 | 0.1 |
| (1,3125) | 1:112:A:TYR:HA | 1:112:A:TYR:HE2 | 7 | 0.1 |
| (1,3116) | 1:63:A:TYR:HD1 | 1:64:A:PRO:HA | 3 | 0.1 |
| (1,3116) | 1:63:A:TYR:HD2 | 1:64:A:PRO:HA | 3 | 0.1 |
| (1,3089) | 1:52:A:VAL:HG21 | 1:77:A:GLN:HE22 | 9 | 0.1 |
| (1,3089) | 1:52:A:VAL:HG22 | 1:77:A:GLN:HE22 | 9 | 0.1 |
| (1,3089) | 1:52:A:VAL:HG23 | 1:77:A:GLN:HE22 | 9 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3026) | 1:219:A:THR:H | 1:219:A:THR:HB | 10 | 0.1 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD2 | 11 | 0.1 |
| (1,2952) | 1:199:A:GLY:H | 1:225:A:LYS:HD3 | 11 | 0.1 |
| (1,2950) | 1:198:A:THR:HA | 1:199:A:GLY:H | 11 | 0.1 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 6 | 0.1 |
| (1,2906) | 1:191:A:THR:HB | 1:192:A:ILE:H | 8 | 0.1 |
| (1,2858) | 1:181:A:GLU:HB2 | 1:183:A:ALA:H | 2 | 0.1 |
| (1,2858) | 1:181:A:GLU:HB3 | 1:183:A:ALA:H | 2 | 0.1 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB1 | 15 | 0.1 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB2 | 15 | 0.1 |
| (1,2812) | 1:175:A:ASN:H | 1:178:A:ALA:HB3 | 15 | 0.1 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB1 | 5 | 0.1 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB2 | 5 | 0.1 |
| (1,2795) | 1:172:A:SER:H | 1:176:A:ALA:HB3 | 5 | 0.1 |
| (1,2790) | 1:172:A:SER:H | 1:172:A:SER:HB3 | 3 | 0.1 |
| (1,2747) | 1:165:A:PHE:H | 1:166:A:ASP:H | 18 | 0.1 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG21 | 9 | 0.1 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG22 | 9 | 0.1 |
| (1,2677) | 1:152:A:LYS:H | 1:153:A:VAL:HG23 | 9 | 0.1 |
| (1,2628) | 1:143:A:VAL:HB | 1:145:A:ALA:H | 10 | 0.1 |
| (1,2607) | 1:142:A:THR:H | 1:147:A:GLY:HA2 | 1 | 0.1 |
| (1,2604) | 1:141:A:GLU:H | 1:142:A:THR:H | 17 | 0.1 |
| (1,2557) | 1:184:A:ILE:HD11 | 1:214:A:ALA:H | 16 | 0.1 |
| (1,2557) | 1:184:A:ILE:HD12 | 1:214:A:ALA:H | 16 | 0.1 |
| (1,2557) | 1:184:A:ILE:HD13 | 1:214:A:ALA:H | 16 | 0.1 |
| (1,2547) | 1:130:A:THR:HG21 | 1:132:A:ASP:H | 2 | 0.1 |
| (1,2547) | 1:130:A:THR:HG22 | 1:132:A:ASP:H | 2 | 0.1 |
| (1,2547) | 1:130:A:THR:HG23 | 1:132:A:ASP:H | 2 | 0.1 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 1 | 0.1 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 14 | 0.1 |
| (1,2515) | 1:123:A:LYS:HG2 | 1:124:A:GLY:H | 20 | 0.1 |
| (1,2500) | 1:120:A:LYS:HE2 | 1:121:A:GLY:H | 20 | 0.1 |
| (1,2500) | 1:120:A:LYS:HE3 | 1:121:A:GLY:H | 20 | 0.1 |
| (1,2498) | 1:110:A:VAL:HG21 | 1:121:A:GLY:H | 4 | 0.1 |
| (1,2498) | 1:110:A:VAL:HG22 | 1:121:A:GLY:H | 4 | 0.1 |
| (1,2498) | 1:110:A:VAL:HG23 | 1:121:A:GLY:H | 4 | 0.1 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 9 | 0.1 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 9 | 0.1 |
| (1,2455) | 1:115:A:ASN:HB2 | 1:117:A:VAL:H | 10 | 0.1 |
| (1,2455) | 1:115:A:ASN:HB3 | 1:117:A:VAL:H | 10 | 0.1 |
| (1,2416) | 1:109:A:ASN:H | 1:109:A:ASN:HD21 | 7 | 0.1 |
| (1,2314) | 1:83:A:GLN:H | 1:83:A:GLN:HB3 | 9 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2201) | 1:59:A:ALA:H | 1:60:A:LYS:HG2 | 8 | 0.1 |
| (1,2199) | 1:58:A:HIS:HB2 | 1:59:A:ALA:H | 17 | 0.1 |
| (1,2194) | 1:58:A:HIS:H | 1:71:A:GLY:HA2 | 16 | 0.1 |
| (1,2181) | 1:55:A:ASN:HB2 | 1:56:A:ALA:H | 11 | 0.1 |
| (1,2152) | 1:52:A:VAL:H | 2:8:B:ILE:HG21 | 7 | 0.1 |
| (1,2152) | 1:52:A:VAL:H | 2:8:B:ILE:HG22 | 7 | 0.1 |
| (1,2152) | 1:52:A:VAL:H | 2:8:B:ILE:HG23 | 7 | 0.1 |
| (1,2143) | 1:50:A:LEU:H | 1:51:A:PRO:HD2 | 12 | 0.1 |
| (1,2136) | 1:101:A:VAL:HG11 | 1:102:A:ARG:HA | 6 | 0.1 |
| (1,2136) | 1:101:A:VAL:HG12 | 1:102:A:ARG:HA | 6 | 0.1 |
| (1,2136) | 1:101:A:VAL:HG13 | 1:102:A:ARG:HA | 6 | 0.1 |
| (1,2136) | 1:101:A:VAL:HG21 | 1:102:A:ARG:HA | 6 | 0.1 |
| (1,2136) | 1:101:A:VAL:HG22 | 1:102:A:ARG:HA | 6 | 0.1 |
| (1,2136) | 1:101:A:VAL:HG23 | 1:102:A:ARG:HA | 6 | 0.1 |
| (1,2120) | 1:74:A:ASP:HA | 1:83:A:GLN:HG3 | 6 | 0.1 |
| (1,2110) | 1:56:A:ALA:HB1 | 1:73:A:VAL:HB | 5 | 0.1 |
| (1,2110) | 1:56:A:ALA:HB2 | 1:73:A:VAL:HB | 5 | 0.1 |
| (1,2110) | 1:56:A:ALA:HB3 | 1:73:A:VAL:HB | 5 | 0.1 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG21 | 17 | 0.1 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG22 | 17 | 0.1 |
| (1,2106) | 1:192:A:ILE:HA | 1:219:A:THR:HG23 | 17 | 0.1 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG21 | 16 | 0.1 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG22 | 16 | 0.1 |
| (1,2099) | 1:116:A:GLN:HB3 | 1:186:A:THR:HG23 | 16 | 0.1 |
| (1,2083) | 1:223:A:THR:HB | 1:224:A:LEU:HB2 | 9 | 0.1 |
| (1,2083) | 1:223:A:THR:HB | 1:224:A:LEU:HB3 | 9 | 0.1 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG21 | 16 | 0.1 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG22 | 16 | 0.1 |
| (1,2046) | 1:169:A:THR:HA | 1:198:A:THR:HG23 | 16 | 0.1 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB2 | 11 | 0.1 |
| (1,1950) | 1:211:A:ALA:HB1 | 1:212:A:LYS:HB3 | 11 | 0.1 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB2 | 11 | 0.1 |
| (1,1950) | 1:211:A:ALA:HB2 | 1:212:A:LYS:HB3 | 11 | 0.1 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB2 | 11 | 0.1 |
| (1,1950) | 1:211:A:ALA:HB3 | 1:212:A:LYS:HB3 | 11 | 0.1 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD2 | 17 | 0.1 |
| (1,1939) | 1:210:A:LYS:H | 1:210:A:LYS:HD3 | 17 | 0.1 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB1 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB2 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG21 | 1:203:A:ALA:HB3 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB1 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB2 | 6 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1846) | 1:202:A:THR:HG22 | 1:203:A:ALA:HB3 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB1 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB2 | 6 | 0.1 |
| (1,1846) | 1:202:A:THR:HG23 | 1:203:A:ALA:HB3 | 6 | 0.1 |
| (1,1824) | 1:201:A:ILE:HG21 | 1:202:A:THR:HA | 3 | 0.1 |
| (1,1824) | 1:201:A:ILE:HG22 | 1:202:A:THR:HA | 3 | 0.1 |
| (1,1824) | 1:201:A:ILE:HG23 | 1:202:A:THR:HA | 3 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 9 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 9 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 9 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 10 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 10 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 10 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 15 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 15 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 15 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB1 | 1:216:A:LEU:H | 16 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB2 | 1:216:A:LEU:H | 16 | 0.1 |
| (1,1774) | 1:213:A:ALA:HB3 | 1:216:A:LEU:H | 16 | 0.1 |
| (1,1765) | 1:170:A:PHE:HB3 | 1:199:A:GLY:HA3 | 12 | 0.1 |
| (1,1757) | 1:169:A:THR:HB | 1:198:A:THR:HB | 11 | 0.1 |
| (1,1740) | 1:169:A:THR:HA | 1:197:A:ALA:HA | 20 | 0.1 |
| (1,1731) | 1:167:A:ASP:HA | 1:196:A:ASN:HB3 | 10 | 0.1 |
| (1,1724) | 1:167:A:ASP:HA | 1:196:A:ASN:HA | 19 | 0.1 |
| (1,1691) | 1:194:A:ILE:HD11 | 1:223:A:THR:H | 9 | 0.1 |
| (1,1691) | 1:194:A:ILE:HD12 | 1:223:A:THR:H | 9 | 0.1 |
| (1,1691) | 1:194:A:ILE:HD13 | 1:223:A:THR:H | 9 | 0.1 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 2 | 0.1 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 2 | 0.1 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 2 | 0.1 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD11 | 18 | 0.1 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD12 | 18 | 0.1 |
| (1,1655) | 1:191:A:THR:H | 1:192:A:ILE:HD13 | 18 | 0.1 |
| (1,1637) | 1:221:A:THR:HB | 1:222:A:ILE:HA | 14 | 0.1 |
| (1,1610) | 1:186:A:THR:HB | 1:187:A:MET:HA | 19 | 0.1 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG21 | 10 | 0.1 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG22 | 10 | 0.1 |
| (1,1605) | 1:116:A:GLN:HE22 | 1:186:A:THR:HG23 | 10 | 0.1 |
| (1,1587) | 1:184:A:ILE:H | 1:185:A:LYS:HE2 | 17 | 0.1 |
| (1,1567) | 1:184:A:ILE:HG21 | 1:189:A:VAL:H | 4 | 0.1 |
| (1,1567) | 1:184:A:ILE:HG22 | 1:189:A:VAL:H | 4 | 0.1 |
| (1,1567) | 1:184:A:ILE:HG23 | 1:189:A:VAL:H | 4 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 7 | 0.1 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 7 | 0.1 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 7 | 0.1 |
| (1,1539) | 1:183:A:ALA:HB1 | 1:188:A:GLY:H | 17 | 0.1 |
| (1,1539) | 1:183:A:ALA:HB2 | 1:188:A:GLY:H | 17 | 0.1 |
| (1,1539) | 1:183:A:ALA:HB3 | 1:188:A:GLY:H | 17 | 0.1 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 16 | 0.1 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 16 | 0.1 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 16 | 0.1 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD11 | 17 | 0.1 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD12 | 17 | 0.1 |
| (1,1493) | 1:180:A:ILE:H | 1:180:A:ILE:HD13 | 17 | 0.1 |
| (1,1469) | 1:50:A:LEU:HB3 | 1:51:A:PRO:HG2 | 9 | 0.1 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB1 | 4 | 0.1 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB2 | 4 | 0.1 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB3 | 4 | 0.1 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB1 | 16 | 0.1 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB2 | 16 | 0.1 |
| (1,1453) | 1:177:A:GLU:H | 1:178:A:ALA:HB3 | 16 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD11 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD12 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD13 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD21 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD22 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD21 | 1:163:A:LEU:HD23 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD11 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD12 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD13 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD21 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD22 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD22 | 1:163:A:LEU:HD23 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD11 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD12 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD13 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD21 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD22 | 18 | 0.1 |
| (1,1341) | 1:119:A:LEU:HD23 | 1:163:A:LEU:HD23 | 18 | 0.1 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 5 | 0.1 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 5 | 0.1 |
| (1,1338) | 1:163:A:LEU:HB2 | 1:164:A:GLU:H | 7 | 0.1 |
| (1,1338) | 1:163:A:LEU:HB3 | 1:164:A:GLU:H | 7 | 0.1 |
| (1,1279) | 1:157:A:LEU:HG | 1:158:A:ASP:H | 3 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1233) | 1:154:A:ILE:HG21 | 1:165:A:PHE:HB2 | 13 | 0.1 |
| (1,1233) | 1:154:A:ILE:HG22 | 1:165:A:PHE:HB2 | 13 | 0.1 |
| (1,1233) | 1:154:A:ILE:HG23 | 1:165:A:PHE:HB2 | 13 | 0.1 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD11 | 16 | 0.1 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD12 | 16 | 0.1 |
| (1,1228) | 1:135:A:PHE:HB3 | 1:154:A:ILE:HD13 | 16 | 0.1 |
| (1,1204) | 1:152:A:LYS:H | 1:152:A:LYS:HG3 | 15 | 0.1 |
| (1,1201) | 1:209:A:LEU:H | 1:210:A:LYS:HE2 | 8 | 0.1 |
| (1,1201) | 1:209:A:LEU:H | 1:210:A:LYS:HE3 | 8 | 0.1 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 12 | 0.1 |
| (1,1196) | 1:136:A:TYR:HA | 1:152:A:LYS:HB3 | 16 | 0.1 |
| (1,1173) | 1:151:A:ALA:HA | 1:152:A:LYS:HA | 9 | 0.1 |
| (1,1173) | 1:151:A:ALA:HA | 1:152:A:LYS:HA | 11 | 0.1 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 15 | 0.1 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 15 | 0.1 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB2 | 18 | 0.1 |
| (1,1165) | 1:141:A:GLU:H | 1:148:A:SER:HB3 | 18 | 0.1 |
| (1,1164) | 1:148:A:SER:HB2 | 1:149:A:ALA:H | 8 | 0.1 |
| (1,1164) | 1:148:A:SER:HB3 | 1:149:A:ALA:H | 8 | 0.1 |
| (1,1155) | 1:141:A:GLU:H | 1:148:A:SER:HA | 2 | 0.1 |
| (1,1138) | 1:145:A:ALA:HB1 | 1:178:A:ALA:HA | 8 | 0.1 |
| (1,1138) | 1:145:A:ALA:HB2 | 1:178:A:ALA:HA | 8 | 0.1 |
| (1,1138) | 1:145:A:ALA:HB3 | 1:178:A:ALA:HA | 8 | 0.1 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG21 | 2 | 0.1 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG22 | 2 | 0.1 |
| (1,1124) | 1:117:A:VAL:HB | 1:142:A:THR:HG23 | 2 | 0.1 |
| (1,1088) | 1:140:A:ILE:HG21 | 1:141:A:GLU:HB3 | 16 | 0.1 |
| (1,1088) | 1:140:A:ILE:HG22 | 1:141:A:GLU:HB3 | 16 | 0.1 |
| (1,1088) | 1:140:A:ILE:HG23 | 1:141:A:GLU:HB3 | 16 | 0.1 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG11 | 6 | 0.1 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG12 | 6 | 0.1 |
| (1,977) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG13 | 6 | 0.1 |
| (1,966) | 1:134:A:VAL:HA | 1:155:A:LYS:HG3 | 18 | 0.1 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE2 | 15 | 0.1 |
| (1,957) | 1:131:A:LYS:HA | 1:131:A:LYS:HE3 | 15 | 0.1 |
| (1,911) | 1:125:A:TRP:HA | 1:134:A:VAL:HB | 19 | 0.1 |
| (1,870) | 1:110:A:VAL:HG11 | 1:122:A:PRO:HA | 8 | 0.1 |
| (1,870) | 1:110:A:VAL:HG12 | 1:122:A:PRO:HA | 8 | 0.1 |
| (1,870) | 1:110:A:VAL:HG13 | 1:122:A:PRO:HA | 8 | 0.1 |
| (1,824) | 1:117:A:VAL:HG21 | 1:141:A:GLU:H | 4 | 0.1 |
| (1,824) | 1:117:A:VAL:HG22 | 1:141:A:GLU:H | 4 | 0.1 |
| (1,824) | 1:117:A:VAL:HG23 | 1:141:A:GLU:H | 4 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,818) | 1:117:A:VAL:HG21 | 1:140:A:ILE:HA | 1 | 0.1 |
| (1,818) | 1:117:A:VAL:HG22 | 1:140:A:ILE:HA | 1 | 0.1 |
| (1,818) | 1:117:A:VAL:HG23 | 1:140:A:ILE:HA | 1 | 0.1 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 8 | 0.1 |
| (1,684) | 1:140:A:ILE:H | 1:150:A:SER:HA | 11 | 0.1 |
| (1,655) | 1:102:A:ARG:HD2 | 1:103:A:THR:H | 8 | 0.1 |
| (1,655) | 1:102:A:ARG:HD3 | 1:103:A:THR:H | 8 | 0.1 |
| (1,625) | 1:99:A:GLU:HA | 1:99:A:GLU:HG2 | 8 | 0.1 |
| (1,625) | 1:99:A:GLU:HA | 1:99:A:GLU:HG3 | 8 | 0.1 |
| (1,619) | 1:98:A:PRO:HB2 | 1:99:A:GLU:HA | 12 | 0.1 |
| (1,603) | 1:94:A:ALA:HB1 | 1:97:A:GLN:HA | 6 | 0.1 |
| (1,603) | 1:94:A:ALA:HB2 | 1:97:A:GLN:HA | 6 | 0.1 |
| (1,603) | 1:94:A:ALA:HB3 | 1:97:A:GLN:HA | 6 | 0.1 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 8 | 0.1 |
| (1,517) | 1:86:A:GLU:HA | 1:86:A:GLU:HG2 | 11 | 0.1 |
| (1,443) | 1:77:A:GLN:HA | 1:78:A:GLY:HA2 | 19 | 0.1 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD11 | 7 | 0.1 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD12 | 7 | 0.1 |
| (1,387) | 1:206:A:ALA:H | 1:222:A:ILE:HD13 | 7 | 0.1 |
| (1,353) | 1:73:A:VAL:HG11 | 1:74:A:ASP:HA | 5 | 0.1 |
| (1,353) | 1:73:A:VAL:HG12 | 1:74:A:ASP:HA | 5 | 0.1 |
| (1,353) | 1:73:A:VAL:HG13 | 1:74:A:ASP:HA | 5 | 0.1 |
| (1,351) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG21 | 19 | 0.1 |
| (1,351) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG22 | 19 | 0.1 |
| (1,351) | 1:125:A:TRP:HB3 | 1:134:A:VAL:HG23 | 19 | 0.1 |
| (1,348) | 1:134:A:VAL:HG21 | 1:155:A:LYS:HB2 | 5 | 0.1 |
| (1,348) | 1:134:A:VAL:HG22 | 1:155:A:LYS:HB2 | 5 | 0.1 |
| (1,348) | 1:134:A:VAL:HG23 | 1:155:A:LYS:HB2 | 5 | 0.1 |
| (1,338) | 1:172:A:SER:HA | 1:173:A:TYR:HA | 9 | 0.1 |
| (1,307) | 1:70:A:THR:HB | 1:72:A:SER:H | 11 | 0.1 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB1 | 11 | 0.1 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB2 | 11 | 0.1 |
| (1,262) | 1:66:A:ASP:HA | 1:67:A:ALA:HB3 | 11 | 0.1 |
| (1,187) | 1:58:A:HIS:HB2 | 1:70:A:THR:H | 12 | 0.1 |
| (1,173) | 1:56:A:ALA:HB1 | 1:57:A:ASP:HB2 | 13 | 0.1 |
| (1,173) | 1:56:A:ALA:HB2 | 1:57:A:ASP:HB2 | 13 | 0.1 |
| (1,173) | 1:56:A:ALA:HB3 | 1:57:A:ASP:HB2 | 13 | 0.1 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG21 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG22 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG21 | 1:198:A:THR:HG23 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG21 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG22 | 7 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|------------------|------------------|----------|---------------|
| (1,91) | 1:169:A:THR:HG22 | 1:198:A:THR:HG23 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG21 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG22 | 7 | 0.1 |
| (1,91) | 1:169:A:THR:HG23 | 1:198:A:THR:HG23 | 7 | 0.1 |
| (1,90) | 1:53:A:THR:HB | 1:55:A:ASN:H | 5 | 0.1 |
| (1,86) | 1:53:A:THR:HB | 1:55:A:ASN:HD21 | 10 | 0.1 |
| (1,51) | 1:122:A:PRO:HD3 | 1:137:A:ASP:HB3 | 8 | 0.1 |
| (1,51) | 1:122:A:PRO:HD3 | 1:137:A:ASP:HB3 | 11 | 0.1 |
| (1,35) | 1:155:A:LYS:HB3 | 1:155:A:LYS:HE2 | 7 | 0.1 |
| (1,9) | 1:47:A:THR:HA | 1:50:A:LEU:H | 8 | 0.1 |

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found