



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 AM UTC

PDB ID : 2LEN / pdb_00002len
BMRB ID : 17260
Title : Solution structure of UCHL1 S18Y variant
Authors : Tse, H.
Deposited on : 2011-06-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

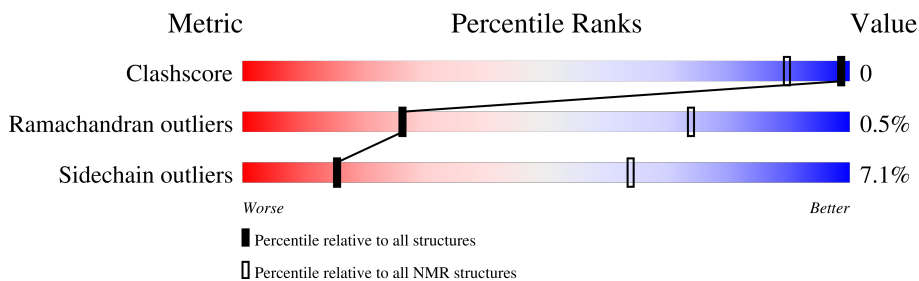
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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 | 231 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:3-A:151, A:160-A:208, A:214-A:222 (207) | 1.11 | 14 |

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3292 atoms, of which 1468 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase isozyme L1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 231 | 3292 | 1148 | 1468 | 322 | 342 | 12 | 0 |

There are 9 discrepancies between the modelled and reference sequences:

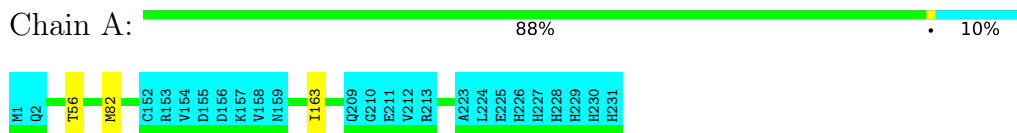
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 18 | TYR | SER | engineered mutation | UNP P09936 |
| A | 224 | LEU | - | expression tag | UNP P09936 |
| A | 225 | GLU | - | expression tag | UNP P09936 |
| A | 226 | HIS | - | expression tag | UNP P09936 |
| A | 227 | HIS | - | expression tag | UNP P09936 |
| A | 228 | HIS | - | expression tag | UNP P09936 |
| A | 229 | HIS | - | expression tag | UNP P09936 |
| A | 230 | HIS | - | expression tag | UNP P09936 |
| A | 231 | HIS | - | expression tag | UNP P09936 |

4 Residue-property plots i

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1

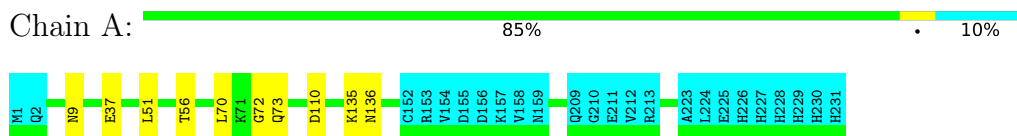


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

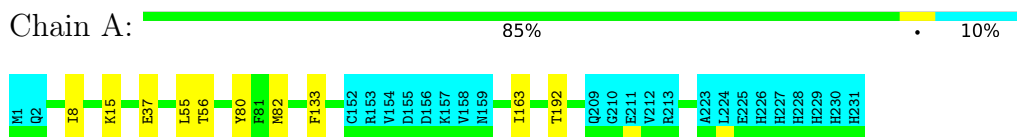
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



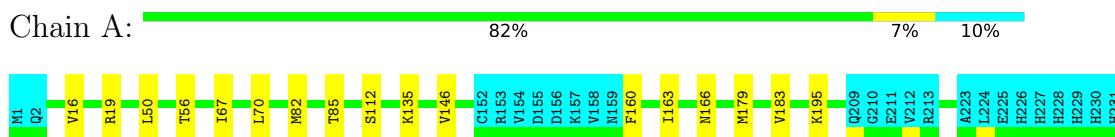
4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



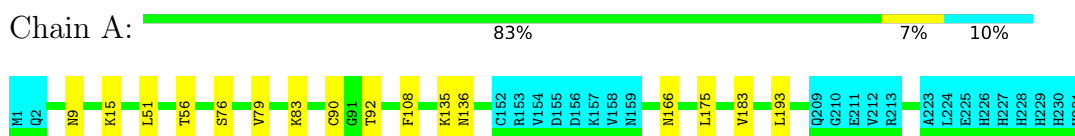
4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



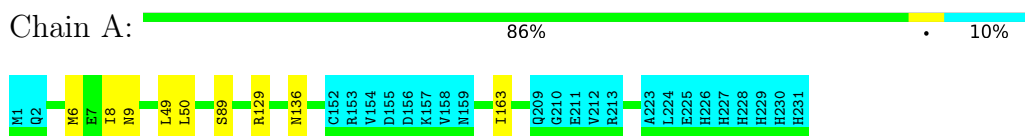
4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



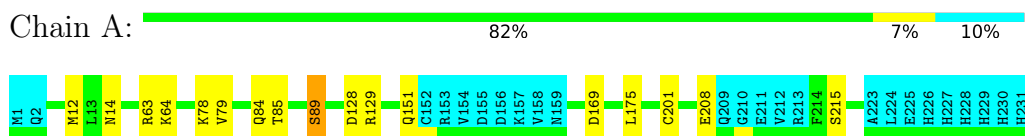
4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



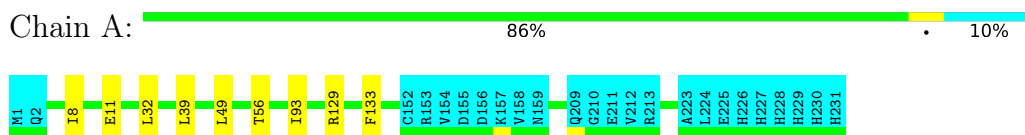
4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



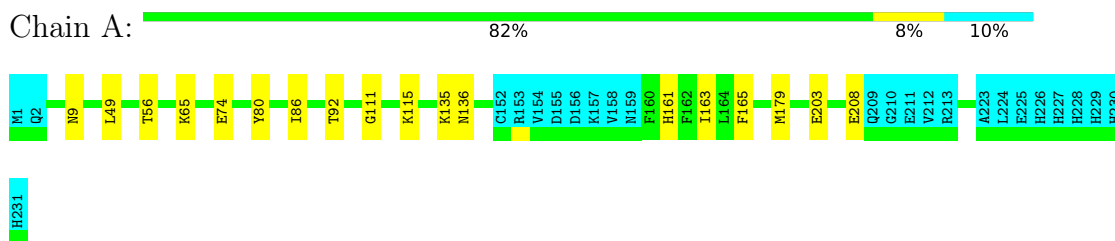
4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



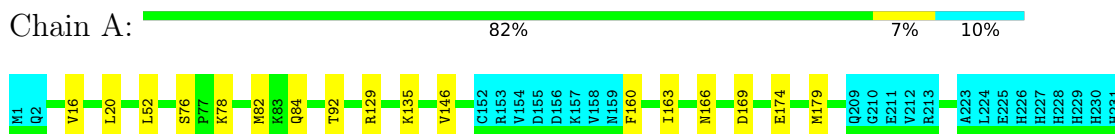
4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



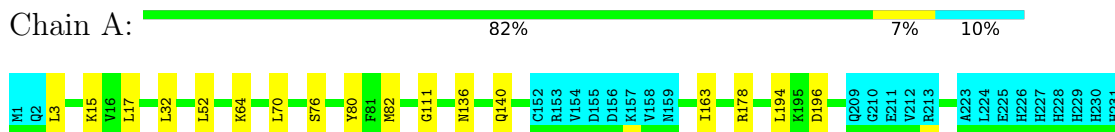
4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



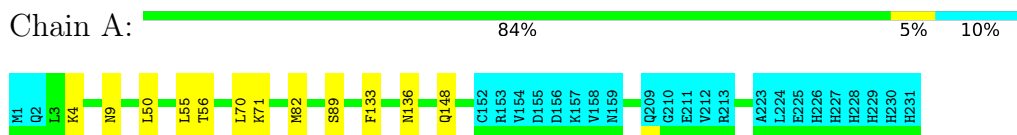
4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



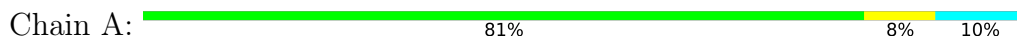
4.2.11 Score per residue for model 11

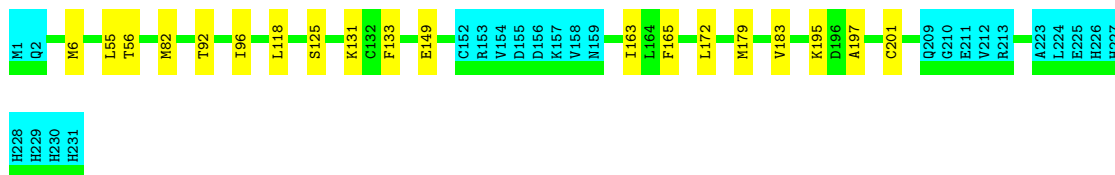
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1

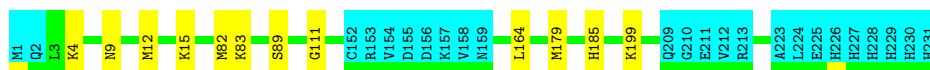




4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1

Chain A: 84% 5% 10%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1

Chain A: 84% 6% 10%



4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1

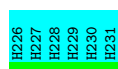
Chain A: 83% 6% 10%



4.2.16 Score per residue for model 16

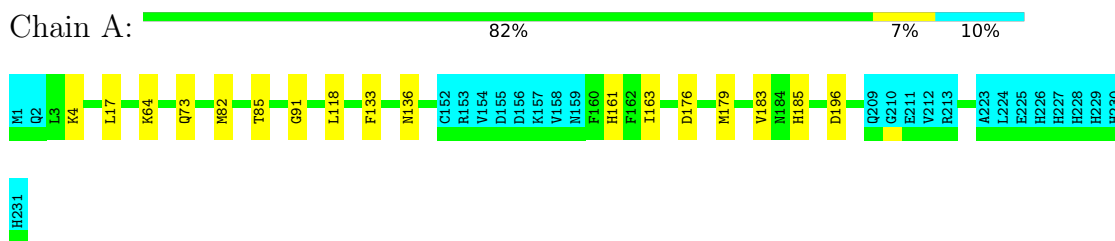
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1

Chain A: 81% 9% 10%



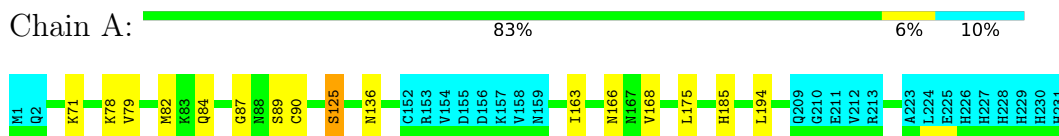
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



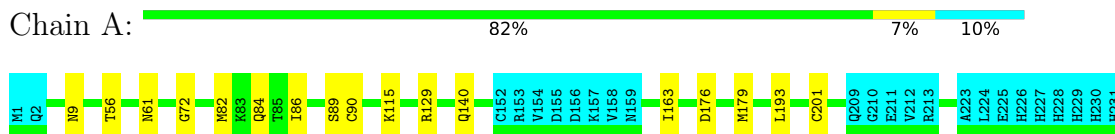
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



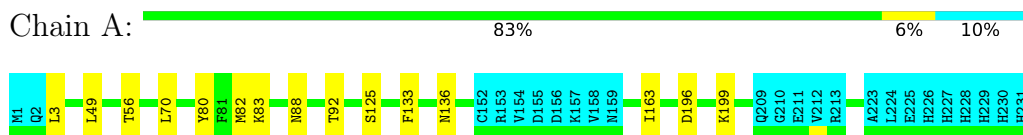
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase isozyme L1



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: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| CYANA | structure solution | |
| Amber | refinement | |
| TALOS | geometry optimization | |

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 | 2 |
| Total number of shifts | 4924 |
| Number of shifts mapped to atoms | 4404 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 520 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 79% |

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 | 0.87±0.01 | 0±0/1653 (0.0± 0.0%) | 1.43±0.02 | 1±1/2230 (0.0± 0.1%) |
| All | All | 0.87 | 0/33060 (0.0%) | 1.43 | 17/44600 (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±0.2 |
| All | All | 0 | 1 |

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 91 | GLY | CA-C-N | 5.42 | 127.80 | 120.38 | 17 | 1 |
| 1 | A | 91 | GLY | C-N-CA | 5.42 | 127.80 | 120.38 | 17 | 1 |
| 1 | A | 86 | ILE | CA-C-N | 5.38 | 126.30 | 122.16 | 19 | 1 |
| 1 | A | 86 | ILE | C-N-CA | 5.38 | 126.30 | 122.16 | 19 | 1 |
| 1 | A | 192 | THR | CA-C-N | 5.32 | 127.72 | 120.54 | 2 | 1 |
| 1 | A | 192 | THR | C-N-CA | 5.32 | 127.72 | 120.54 | 2 | 1 |
| 1 | A | 201 | CYS | CA-C-N | 5.31 | 127.66 | 120.65 | 12 | 2 |
| 1 | A | 201 | CYS | C-N-CA | 5.31 | 127.66 | 120.65 | 12 | 2 |
| 1 | A | 121 | THR | CA-C-N | 5.24 | 128.69 | 120.82 | 14 | 1 |
| 1 | A | 121 | THR | C-N-CA | 5.24 | 128.69 | 120.82 | 14 | 1 |
| 1 | A | 71 | LYS | CA-C-N | 5.11 | 125.58 | 120.98 | 11 | 1 |
| 1 | A | 71 | LYS | C-N-CA | 5.11 | 125.58 | 120.98 | 11 | 1 |
| 1 | A | 178 | ARG | CA-C-N | 5.09 | 127.58 | 120.65 | 10 | 1 |
| 1 | A | 178 | ARG | C-N-CA | 5.09 | 127.58 | 120.65 | 10 | 1 |
| 1 | A | 125 | SER | N-CA-C | 5.04 | 112.76 | 108.22 | 18 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 129 | ARG | Sidechain | 1 |

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 1620 | 1315 | 1602 | 1±1 |
| All | All | 32400 | 26300 | 32040 | 12 |

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 0.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:VAL:HG22 | 1:A:146:VAL:HG11 | 0.61 | 1.71 | 15 | 4 |
| 1:A:165:PHE:CZ | 1:A:197:ALA:HB2 | 0.54 | 2.38 | 12 | 1 |
| 1:A:8:ILE:HG21 | 1:A:50:LEU:HD21 | 0.48 | 1.85 | 5 | 1 |
| 1:A:52:LEU:HD11 | 1:A:160:PHE:CD1 | 0.47 | 2.45 | 9 | 1 |
| 1:A:67:ILE:HG22 | 1:A:183:VAL:CG2 | 0.46 | 2.39 | 3 | 1 |
| 1:A:12:MET:O | 1:A:16:VAL:HG23 | 0.45 | 2.11 | 15 | 2 |
| 1:A:165:PHE:CE2 | 1:A:172:LEU:HD13 | 0.43 | 2.49 | 12 | 1 |
| 1:A:79:VAL:CG1 | 1:A:168:VAL:HG21 | 0.41 | 2.45 | 18 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|---------------|-------------|------------|-------------|----|
| 1 | A | 207/231 (90%) | 193±3 (93±1%) | 13±3 (6±1%) | 1±1 (1±0%) | 26 | 74 |
| All | All | 4140/4620 (90%) | 3855 (93%) | 264 (6%) | 21 (1%) | 26 | 74 |

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 89 | SER | 4 |
| 1 | A | 111 | GLY | 4 |
| 1 | A | 90 | CYS | 3 |
| 1 | A | 72 | GLY | 2 |
| 1 | A | 83 | LYS | 2 |
| 1 | A | 110 | ASP | 1 |
| 1 | A | 8 | ILE | 1 |
| 1 | A | 112 | SER | 1 |
| 1 | A | 32 | LEU | 1 |
| 1 | A | 87 | GLY | 1 |
| 1 | A | 88 | ASN | 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 | 174/196 (89%) | 162±3 (93±2%) | 12±3 (7±2%) | 15 | 64 |
| All | All | 3480/3920 (89%) | 3234 (93%) | 246 (7%) | 15 | 64 |

All 83 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 | 82 | MET | 14 |
| 1 | A | 163 | ILE | 14 |
| 1 | A | 56 | THR | 13 |
| 1 | A | 136 | ASN | 10 |
| 1 | A | 9 | ASN | 8 |
| 1 | A | 179 | MET | 8 |
| 1 | A | 133 | PHE | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 92 | THR | 7 |
| 1 | A | 49 | LEU | 6 |
| 1 | A | 70 | LEU | 5 |
| 1 | A | 135 | LYS | 5 |
| 1 | A | 15 | LYS | 5 |
| 1 | A | 55 | LEU | 5 |
| 1 | A | 125 | SER | 5 |
| 1 | A | 80 | TYR | 4 |
| 1 | A | 85 | THR | 4 |
| 1 | A | 166 | ASN | 4 |
| 1 | A | 76 | SER | 4 |
| 1 | A | 183 | VAL | 4 |
| 1 | A | 129 | ARG | 4 |
| 1 | A | 84 | GLN | 4 |
| 1 | A | 73 | GLN | 3 |
| 1 | A | 175 | LEU | 3 |
| 1 | A | 64 | LYS | 3 |
| 1 | A | 78 | LYS | 3 |
| 1 | A | 89 | SER | 3 |
| 1 | A | 32 | LEU | 3 |
| 1 | A | 161 | HIS | 3 |
| 1 | A | 196 | ASP | 3 |
| 1 | A | 4 | LYS | 3 |
| 1 | A | 118 | LEU | 3 |
| 1 | A | 185 | HIS | 3 |
| 1 | A | 37 | GLU | 2 |
| 1 | A | 51 | LEU | 2 |
| 1 | A | 50 | LEU | 2 |
| 1 | A | 195 | LYS | 2 |
| 1 | A | 79 | VAL | 2 |
| 1 | A | 83 | LYS | 2 |
| 1 | A | 193 | LEU | 2 |
| 1 | A | 6 | MET | 2 |
| 1 | A | 12 | MET | 2 |
| 1 | A | 169 | ASP | 2 |
| 1 | A | 208 | GLU | 2 |
| 1 | A | 115 | LYS | 2 |
| 1 | A | 20 | LEU | 2 |
| 1 | A | 3 | LEU | 2 |
| 1 | A | 17 | LEU | 2 |
| 1 | A | 140 | GLN | 2 |
| 1 | A | 194 | LEU | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 148 | GLN | 2 |
| 1 | A | 131 | LYS | 2 |
| 1 | A | 149 | GLU | 2 |
| 1 | A | 199 | LYS | 2 |
| 1 | A | 176 | ASP | 2 |
| 1 | A | 19 | ARG | 1 |
| 1 | A | 160 | PHE | 1 |
| 1 | A | 108 | PHE | 1 |
| 1 | A | 14 | ASN | 1 |
| 1 | A | 63 | ARG | 1 |
| 1 | A | 128 | ASP | 1 |
| 1 | A | 151 | GLN | 1 |
| 1 | A | 201 | CYS | 1 |
| 1 | A | 215 | SER | 1 |
| 1 | A | 8 | ILE | 1 |
| 1 | A | 11 | GLU | 1 |
| 1 | A | 39 | LEU | 1 |
| 1 | A | 93 | ILE | 1 |
| 1 | A | 65 | LYS | 1 |
| 1 | A | 74 | GLU | 1 |
| 1 | A | 86 | ILE | 1 |
| 1 | A | 165 | PHE | 1 |
| 1 | A | 203 | GLU | 1 |
| 1 | A | 174 | GLU | 1 |
| 1 | A | 52 | LEU | 1 |
| 1 | A | 96 | ILE | 1 |
| 1 | A | 164 | LEU | 1 |
| 1 | A | 109 | GLU | 1 |
| 1 | A | 88 | ASN | 1 |
| 1 | A | 123 | LYS | 1 |
| 1 | A | 139 | ILE | 1 |
| 1 | A | 71 | LYS | 1 |
| 1 | A | 90 | CYS | 1 |
| 1 | A | 61 | 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 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

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 | 2462 |
| Number of shifts mapped to atoms | 2202 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 260 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 6 |

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

- No matching atom found in the structure. All 260 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 2 | GLN | HB3 | 2.066 | 0.020 | 2 |
| 1 | A | 2 | GLN | HG3 | 2.309 | 0.020 | 2 |
| 1 | A | 3 | LEU | HB3 | 1.353 | 0.020 | 2 |
| 1 | A | 5 | PRO | HB3 | 1.86 | 0.020 | 2 |
| 1 | A | 6 | MET | HB3 | 1.958 | 0.020 | 2 |
| 1 | A | 6 | MET | HG3 | 2.324 | 0.020 | 2 |
| 1 | A | 7 | GLU | HB3 | 1.774 | 0.020 | 2 |
| 1 | A | 7 | GLU | HG3 | 2.143 | 0.020 | 2 |
| 1 | A | 8 | ILE | HG13 | 0.324 | 0.020 | 2 |
| 1 | A | 9 | ASN | HB3 | 2.816 | 0.020 | 2 |
| 1 | A | 10 | PRO | HB3 | 2.233 | 0.020 | 1 |
| 1 | A | 11 | GLU | HB3 | 1.992 | 0.020 | 2 |
| 1 | A | 11 | GLU | HG3 | 2.226 | 0.020 | 2 |
| 1 | A | 13 | LEU | HB3 | 1.286 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 14 | ASN | HB3 | 2.788 | 0.020 | 2 |
| 1 | A | 15 | LYS | HB3 | 1.85 | 0.020 | 2 |
| 1 | A | 15 | LYS | HD3 | 1.685 | 0.020 | 2 |
| 1 | A | 15 | LYS | HE3 | 2.995 | 0.020 | 2 |
| 1 | A | 15 | LYS | HG3 | 1.521 | 0.020 | 2 |
| 1 | A | 17 | LEU | HB3 | 2.086 | 0.020 | 2 |
| 1 | A | 18 | TYR | HB3 | 3.247 | 0.020 | 2 |
| 1 | A | 19 | ARG | HB3 | 1.937 | 0.020 | 2 |
| 1 | A | 19 | ARG | HD3 | 3.26 | 0.020 | 2 |
| 1 | A | 19 | ARG | HG3 | 1.883 | 0.020 | 2 |
| 1 | A | 20 | LEU | HB3 | 1.934 | 0.020 | 2 |
| 1 | A | 21 | GLY | HA3 | 4.037 | 0.020 | 2 |
| 1 | A | 24 | GLY | HA3 | 4.12 | 0.020 | 2 |
| 1 | A | 25 | GLN | HB3 | 2.101 | 0.020 | 1 |
| 1 | A | 25 | GLN | HG3 | 2.292 | 0.020 | 2 |
| 1 | A | 26 | TRP | HB3 | 2.645 | 0.020 | 2 |
| 1 | A | 27 | ARG | HB3 | 1.83 | 0.020 | 2 |
| 1 | A | 27 | ARG | HD3 | 3.158 | 0.020 | 2 |
| 1 | A | 27 | ARG | HG3 | 1.59 | 0.020 | 1 |
| 1 | A | 28 | PHE | HB3 | 3.002 | 0.020 | 2 |
| 1 | A | 30 | ASP | HB3 | 2.551 | 0.020 | 2 |
| 1 | A | 32 | LEU | HB3 | 1.665 | 0.020 | 2 |
| 1 | A | 33 | GLY | HA3 | 4.093 | 0.020 | 2 |
| 1 | A | 34 | LEU | HB3 | 1.523 | 0.020 | 2 |
| 1 | A | 35 | GLU | HB3 | 2.224 | 0.020 | 1 |
| 1 | A | 35 | GLU | HG3 | 2.334 | 0.020 | 2 |
| 1 | A | 36 | GLU | HB3 | 1.998 | 0.020 | 2 |
| 1 | A | 36 | GLU | HG3 | 2.265 | 0.020 | 2 |
| 1 | A | 37 | GLU | HB3 | 2.038 | 0.020 | 2 |
| 1 | A | 37 | GLU | HG3 | 2.294 | 0.020 | 2 |
| 1 | A | 38 | SER | HB3 | 3.791 | 0.020 | 2 |
| 1 | A | 39 | LEU | HB3 | 1.755 | 0.020 | 1 |
| 1 | A | 40 | GLY | HA3 | 4.091 | 0.020 | 2 |
| 1 | A | 41 | SER | HB3 | 3.996 | 0.020 | 2 |
| 1 | A | 43 | PRO | HB3 | 2.275 | 0.020 | 2 |
| 1 | A | 43 | PRO | HG3 | 2.025 | 0.020 | 2 |
| 1 | A | 45 | PRO | HB3 | 2.503 | 0.020 | 1 |
| 1 | A | 45 | PRO | HG3 | 2.02 | 0.020 | 1 |
| 1 | A | 47 | CYS | HB3 | 3.233 | 0.020 | 2 |
| 1 | A | 49 | LEU | HB3 | 1.64 | 0.020 | 2 |
| 1 | A | 50 | LEU | HB3 | 3.097 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 52 | LEU | HB3 | 2.305 | 0.020 | 2 |
| 1 | A | 53 | PHE | HB3 | 2.948 | 0.020 | 2 |
| 1 | A | 55 | LEU | HB3 | 1.564 | 0.020 | 2 |
| 1 | A | 58 | GLN | HB3 | 2.433 | 0.020 | 2 |
| 1 | A | 58 | GLN | HG3 | 2.707 | 0.020 | 2 |
| 1 | A | 59 | HIS | HB3 | 3.536 | 0.020 | 2 |
| 1 | A | 60 | GLU | HB3 | 2.118 | 0.020 | 2 |
| 1 | A | 60 | GLU | HG3 | 2.414 | 0.020 | 2 |
| 1 | A | 61 | ASN | HB3 | 2.918 | 0.020 | 2 |
| 1 | A | 62 | PHE | HB3 | 3.252 | 0.020 | 2 |
| 1 | A | 64 | LYS | HB3 | 1.926 | 0.020 | 2 |
| 1 | A | 64 | LYS | HD3 | 1.703 | 0.020 | 2 |
| 1 | A | 64 | LYS | HE3 | 2.968 | 0.020 | 2 |
| 1 | A | 64 | LYS | HG3 | 1.415 | 0.020 | 2 |
| 1 | A | 65 | LYS | HB3 | 1.883 | 0.020 | 2 |
| 1 | A | 65 | LYS | HD3 | 1.672 | 0.020 | 2 |
| 1 | A | 65 | LYS | HE3 | 2.961 | 0.020 | 2 |
| 1 | A | 65 | LYS | HG3 | 1.338 | 0.020 | 2 |
| 1 | A | 67 | ILE | HG13 | 0.83 | 0.020 | 2 |
| 1 | A | 68 | GLU | HB3 | 2.117 | 0.020 | 2 |
| 1 | A | 68 | GLU | HG3 | 2.405 | 0.020 | 2 |
| 1 | A | 69 | GLU | HB3 | 2.131 | 0.020 | 2 |
| 1 | A | 70 | LEU | HB3 | 1.765 | 0.020 | 2 |
| 1 | A | 71 | LYS | HB3 | 1.913 | 0.020 | 2 |
| 1 | A | 71 | LYS | HD3 | 1.738 | 0.020 | 2 |
| 1 | A | 71 | LYS | HE3 | 3.004 | 0.020 | 2 |
| 1 | A | 71 | LYS | HG3 | 1.495 | 0.020 | 2 |
| 1 | A | 72 | GLY | HA3 | 3.898 | 0.020 | 2 |
| 1 | A | 73 | GLN | HB3 | 2.036 | 0.020 | 2 |
| 1 | A | 73 | GLN | HG3 | 2.284 | 0.020 | 2 |
| 1 | A | 74 | GLU | HB3 | 1.824 | 0.020 | 2 |
| 1 | A | 74 | GLU | HG3 | 2.003 | 0.020 | 2 |
| 1 | A | 76 | SER | HB3 | 4.377 | 0.020 | 2 |
| 1 | A | 77 | PRO | HB3 | 2.361 | 0.020 | 1 |
| 1 | A | 77 | PRO | HD3 | 3.948 | 0.020 | 2 |
| 1 | A | 77 | PRO | HG3 | 2.072 | 0.020 | 2 |
| 1 | A | 78 | LYS | HB3 | 1.81 | 0.020 | 2 |
| 1 | A | 78 | LYS | HD3 | 1.663 | 0.020 | 2 |
| 1 | A | 78 | LYS | HE3 | 2.959 | 0.020 | 2 |
| 1 | A | 78 | LYS | HG3 | 1.387 | 0.020 | 2 |
| 1 | A | 80 | TYR | HB3 | 2.822 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 81 | PHE | HB3 | 3.389 | 0.020 | 2 |
| 1 | A | 82 | MET | HB3 | 1.818 | 0.020 | 1 |
| 1 | A | 82 | MET | HG3 | 2.34 | 0.020 | 2 |
| 1 | A | 83 | LYS | HB3 | 1.284 | 0.020 | 2 |
| 1 | A | 83 | LYS | HE3 | 3.043 | 0.020 | 2 |
| 1 | A | 86 | ILE | HG13 | 1.593 | 0.020 | 2 |
| 1 | A | 87 | GLY | HA3 | 4.069 | 0.020 | 2 |
| 1 | A | 88 | ASN | HB3 | 2.955 | 0.020 | 2 |
| 1 | A | 89 | SER | HB3 | 4.026 | 0.020 | 2 |
| 1 | A | 90 | CYS | HB3 | 2.906 | 0.020 | 2 |
| 1 | A | 91 | GLY | HA3 | 3.893 | 0.020 | 2 |
| 1 | A | 93 | ILE | HG13 | 1.122 | 0.020 | 2 |
| 1 | A | 94 | GLY | HA3 | 3.965 | 0.020 | 2 |
| 1 | A | 96 | ILE | HG13 | 2.001 | 0.020 | 2 |
| 1 | A | 97 | HIS | HB3 | 3.0 | 0.020 | 2 |
| 1 | A | 101 | ASN | HB3 | 2.911 | 0.020 | 1 |
| 1 | A | 102 | ASN | HB3 | 2.589 | 0.020 | 1 |
| 1 | A | 103 | GLN | HB3 | 2.408 | 0.020 | 2 |
| 1 | A | 103 | GLN | HG3 | 2.58 | 0.020 | 2 |
| 1 | A | 104 | ASP | HB3 | 2.738 | 0.020 | 2 |
| 1 | A | 105 | LYS | HB3 | 1.518 | 0.020 | 1 |
| 1 | A | 105 | LYS | HD3 | 1.667 | 0.020 | 2 |
| 1 | A | 105 | LYS | HE3 | 3.147 | 0.020 | 2 |
| 1 | A | 105 | LYS | HG3 | 1.267 | 0.020 | 2 |
| 1 | A | 106 | LEU | HB3 | 1.041 | 0.020 | 2 |
| 1 | A | 107 | GLY | HA3 | 4.365 | 0.020 | 1 |
| 1 | A | 108 | PHE | HB3 | 2.796 | 0.020 | 2 |
| 1 | A | 109 | GLU | HB3 | 2.125 | 0.020 | 2 |
| 1 | A | 109 | GLU | HG3 | 2.389 | 0.020 | 2 |
| 1 | A | 110 | ASP | HB3 | 2.625 | 0.020 | 2 |
| 1 | A | 111 | GLY | HA3 | 3.811 | 0.020 | 2 |
| 1 | A | 112 | SER | HB3 | 3.867 | 0.020 | 2 |
| 1 | A | 114 | LEU | HB3 | 1.602 | 0.020 | 2 |
| 1 | A | 115 | LYS | HB3 | 1.612 | 0.020 | 2 |
| 1 | A | 115 | LYS | HD3 | 1.299 | 0.020 | 2 |
| 1 | A | 115 | LYS | HE3 | 2.771 | 0.020 | 2 |
| 1 | A | 115 | LYS | HG3 | 1.129 | 0.020 | 2 |
| 1 | A | 116 | GLN | HB3 | 2.142 | 0.020 | 2 |
| 1 | A | 116 | GLN | HG3 | 2.463 | 0.020 | 2 |
| 1 | A | 117 | PHE | HB3 | 3.29 | 0.020 | 1 |
| 1 | A | 118 | LEU | HB3 | 1.74 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 119 | SER | HB3 | 3.946 | 0.020 | 2 |
| 1 | A | 120 | GLU | HB3 | 2.086 | 0.020 | 2 |
| 1 | A | 120 | GLU | HG3 | 2.208 | 0.020 | 2 |
| 1 | A | 122 | GLU | HB3 | 2.46 | 0.020 | 1 |
| 1 | A | 122 | GLU | HG3 | 2.233 | 0.020 | 2 |
| 1 | A | 123 | LYS | HB3 | 2.066 | 0.020 | 2 |
| 1 | A | 123 | LYS | HD3 | 1.675 | 0.020 | 2 |
| 1 | A | 123 | LYS | HE3 | 2.964 | 0.020 | 2 |
| 1 | A | 123 | LYS | HG3 | 1.366 | 0.020 | 2 |
| 1 | A | 124 | MET | HB3 | 2.018 | 0.020 | 2 |
| 1 | A | 124 | MET | HG3 | 2.718 | 0.020 | 2 |
| 1 | A | 125 | SER | HB3 | 4.148 | 0.020 | 2 |
| 1 | A | 126 | PRO | HB3 | 1.948 | 0.020 | 2 |
| 1 | A | 127 | GLU | HB3 | 1.954 | 0.020 | 2 |
| 1 | A | 127 | GLU | HG3 | 2.464 | 0.020 | 2 |
| 1 | A | 128 | ASP | HB3 | 2.856 | 0.020 | 2 |
| 1 | A | 129 | ARG | HB3 | 1.915 | 0.020 | 2 |
| 1 | A | 129 | ARG | HD3 | 3.037 | 0.020 | 2 |
| 1 | A | 129 | ARG | HG3 | 1.724 | 0.020 | 2 |
| 1 | A | 131 | LYS | HB3 | 1.984 | 0.020 | 2 |
| 1 | A | 131 | LYS | HE3 | 2.962 | 0.020 | 2 |
| 1 | A | 132 | CYS | HB3 | 3.089 | 0.020 | 1 |
| 1 | A | 133 | PHE | HB3 | 3.507 | 0.020 | 1 |
| 1 | A | 134 | GLU | HB3 | 2.221 | 0.020 | 2 |
| 1 | A | 134 | GLU | HG3 | 2.643 | 0.020 | 2 |
| 1 | A | 135 | LYS | HB3 | 2.055 | 0.020 | 2 |
| 1 | A | 135 | LYS | HD3 | 1.686 | 0.020 | 2 |
| 1 | A | 135 | LYS | HE3 | 2.982 | 0.020 | 2 |
| 1 | A | 135 | LYS | HG3 | 1.574 | 0.020 | 2 |
| 1 | A | 136 | ASN | HB3 | 2.901 | 0.020 | 2 |
| 1 | A | 137 | GLU | HB3 | 1.98 | 0.020 | 2 |
| 1 | A | 137 | GLU | HG3 | 2.34 | 0.020 | 2 |
| 1 | A | 139 | ILE | HG13 | 1.555 | 0.020 | 2 |
| 1 | A | 140 | GLN | HB3 | 2.002 | 0.020 | 2 |
| 1 | A | 140 | GLN | HG3 | 2.289 | 0.020 | 2 |
| 1 | A | 143 | HIS | HB3 | 3.476 | 0.020 | 2 |
| 1 | A | 148 | GLN | HB3 | 2.194 | 0.020 | 2 |
| 1 | A | 148 | GLN | HG3 | 2.54 | 0.020 | 2 |
| 1 | A | 149 | GLU | HB3 | 2.136 | 0.020 | 2 |
| 1 | A | 149 | GLU | HG3 | 2.577 | 0.020 | 2 |
| 1 | A | 150 | GLY | HA3 | 4.31 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 151 | GLN | HB3 | 1.99 | 0.020 | 2 |
| 1 | A | 151 | GLN | HG3 | 2.315 | 0.020 | 2 |
| 1 | A | 152 | CYS | HB3 | 2.807 | 0.020 | 2 |
| 1 | A | 153 | ARG | HB3 | 1.779 | 0.020 | 2 |
| 1 | A | 153 | ARG | HD3 | 3.177 | 0.020 | 2 |
| 1 | A | 153 | ARG | HG3 | 1.593 | 0.020 | 2 |
| 1 | A | 155 | ASP | HB3 | 2.831 | 0.020 | 2 |
| 1 | A | 156 | ASP | HB3 | 2.723 | 0.020 | 2 |
| 1 | A | 157 | LYS | HB3 | 1.809 | 0.020 | 2 |
| 1 | A | 157 | LYS | HD3 | 1.599 | 0.020 | 2 |
| 1 | A | 157 | LYS | HE3 | 2.95 | 0.020 | 2 |
| 1 | A | 157 | LYS | HG3 | 1.364 | 0.020 | 2 |
| 1 | A | 160 | PHE | HB3 | 2.796 | 0.020 | 2 |
| 1 | A | 161 | HIS | HB3 | 2.511 | 0.020 | 2 |
| 1 | A | 163 | ILE | HG13 | 1.196 | 0.020 | 2 |
| 1 | A | 165 | PHE | HB3 | 2.821 | 0.020 | 2 |
| 1 | A | 166 | ASN | HB3 | 2.853 | 0.020 | 2 |
| 1 | A | 167 | ASN | HB3 | 2.701 | 0.020 | 2 |
| 1 | A | 169 | ASP | HB3 | 3.312 | 0.020 | 2 |
| 1 | A | 170 | GLY | HA3 | 4.115 | 0.020 | 1 |
| 1 | A | 171 | HIS | HB3 | 2.973 | 0.020 | 2 |
| 1 | A | 173 | TYR | HB3 | 2.806 | 0.020 | 1 |
| 1 | A | 174 | GLU | HB3 | 2.173 | 0.020 | 2 |
| 1 | A | 175 | LEU | HB3 | 1.537 | 0.020 | 2 |
| 1 | A | 176 | ASP | HB3 | 2.765 | 0.020 | 2 |
| 1 | A | 177 | GLY | HA3 | 3.961 | 0.020 | 2 |
| 1 | A | 180 | PRO | HB3 | 2.129 | 0.020 | 2 |
| 1 | A | 181 | PHE | HB3 | 3.303 | 0.020 | 2 |
| 1 | A | 182 | PRO | HB3 | 1.873 | 0.020 | 2 |
| 1 | A | 182 | PRO | HG3 | 1.595 | 0.020 | 2 |
| 1 | A | 184 | ASN | HB3 | 3.089 | 0.020 | 2 |
| 1 | A | 185 | HIS | HB3 | 3.593 | 0.020 | 2 |
| 1 | A | 186 | GLY | HA3 | 4.552 | 0.020 | 2 |
| 1 | A | 188 | SER | HB3 | 3.737 | 0.020 | 2 |
| 1 | A | 189 | SER | HB3 | 4.06 | 0.020 | 2 |
| 1 | A | 190 | GLU | HB3 | 2.151 | 0.020 | 2 |
| 1 | A | 190 | GLU | HG3 | 2.415 | 0.020 | 2 |
| 1 | A | 191 | ASP | HB3 | 2.717 | 0.020 | 2 |
| 1 | A | 193 | LEU | HB3 | 1.734 | 0.020 | 2 |
| 1 | A | 194 | LEU | HB3 | 1.766 | 0.020 | 1 |
| 1 | A | 195 | LYS | HB3 | 1.752 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 195 | LYS | HD3 | 1.638 | 0.020 | 2 |
| 1 | A | 195 | LYS | HE3 | 2.935 | 0.020 | 2 |
| 1 | A | 195 | LYS | HG3 | 1.352 | 0.020 | 2 |
| 1 | A | 196 | ASP | HB3 | 2.644 | 0.020 | 2 |
| 1 | A | 199 | LYS | HB3 | 1.913 | 0.020 | 2 |
| 1 | A | 199 | LYS | HD3 | 1.661 | 0.020 | 2 |
| 1 | A | 199 | LYS | HE3 | 2.99 | 0.020 | 2 |
| 1 | A | 199 | LYS | HG3 | 2.011 | 0.020 | 2 |
| 1 | A | 201 | CYS | HB3 | 3.06 | 0.020 | 2 |
| 1 | A | 203 | GLU | HB3 | 2.451 | 0.020 | 2 |
| 1 | A | 203 | GLU | HG3 | 2.59 | 0.020 | 2 |
| 1 | A | 204 | PHE | HB3 | 3.521 | 0.020 | 2 |
| 1 | A | 206 | GLU | HB3 | 2.008 | 0.020 | 2 |
| 1 | A | 206 | GLU | HG3 | 2.326 | 0.020 | 2 |
| 1 | A | 207 | ARG | HB3 | 2.049 | 0.020 | 2 |
| 1 | A | 207 | ARG | HD3 | 3.157 | 0.020 | 2 |
| 1 | A | 207 | ARG | HG3 | 1.819 | 0.020 | 2 |
| 1 | A | 208 | GLU | HB3 | 2.412 | 0.020 | 2 |
| 1 | A | 208 | GLU | HG3 | 2.443 | 0.020 | 2 |
| 1 | A | 209 | GLN | HB3 | 2.205 | 0.020 | 2 |
| 1 | A | 209 | GLN | HG3 | 2.409 | 0.020 | 2 |
| 1 | A | 210 | GLY | HA3 | 4.05 | 0.020 | 2 |
| 1 | A | 211 | GLU | HB3 | 2.261 | 0.020 | 1 |
| 1 | A | 211 | GLU | HG3 | 2.174 | 0.020 | 2 |
| 1 | A | 213 | ARG | HB3 | 1.891 | 0.020 | 2 |
| 1 | A | 213 | ARG | HD3 | 3.225 | 0.020 | 2 |
| 1 | A | 213 | ARG | HG3 | 1.718 | 0.020 | 2 |
| 1 | A | 214 | PHE | HB3 | 3.093 | 0.020 | 2 |
| 1 | A | 215 | SER | HB3 | 3.919 | 0.020 | 2 |
| 1 | A | 219 | LEU | HB3 | 0.768 | 0.020 | 2 |
| 1 | A | 220 | CYS | HB3 | 2.797 | 0.020 | 2 |
| 1 | A | 221 | LYS | HB3 | 1.05 | 0.020 | 1 |
| 1 | A | 221 | LYS | HD3 | 1.188 | 0.020 | 2 |
| 1 | A | 221 | LYS | HE3 | 2.662 | 0.020 | 2 |
| 1 | A | 221 | LYS | HG3 | 0.568 | 0.020 | 2 |
| 1 | A | 224 | LEU | HB3 | 1.501 | 0.020 | 2 |
| 1 | A | 225 | GLU | HB3 | 1.837 | 0.020 | 2 |
| 1 | A | 225 | GLU | HG3 | 2.14 | 0.020 | 2 |
| 1 | A | 226 | HIS | HB3 | 3.041 | 0.020 | 2 |
| 1 | A | 229 | HIS | HB3 | 3.099 | 0.020 | 2 |
| 1 | A | 230 | HIS | HB3 | 3.118 | 0.020 | 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 |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 229 | -0.18 ± 0.06 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 208 | 0.14 ± 0.14 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 228 | -0.07 ± 0.09 | None needed (< 0.5 ppm) |
| ^{15}N | 217 | 0.05 ± 0.18 | 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 79%, i.e. 2224 atoms were assigned a chemical shift out of a possible 2803. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 1018/1031 (99%) | 410/419 (98%) | 412/414 (100%) | 196/198 (99%) |
| Sidechain | 1204/1561 (77%) | 842/1013 (83%) | 347/492 (71%) | 15/56 (27%) |
| Aromatic | 2/211 (1%) | 1/107 (1%) | 0/97 (0%) | 1/7 (14%) |
| Overall | 2224/2803 (79%) | 1253/1539 (81%) | 759/1003 (76%) | 212/261 (81%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2462 atoms were assigned a chemical shift out of a possible 3142. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 1127/1152 (98%) | 453/468 (97%) | 457/462 (99%) | 217/222 (98%) |
| Sidechain | 1333/1737 (77%) | 930/1125 (83%) | 385/546 (71%) | 18/66 (27%) |
| Aromatic | 2/253 (1%) | 1/131 (1%) | 0/109 (0%) | 1/13 (8%) |
| Overall | 2462/3142 (78%) | 1384/1724 (80%) | 842/1117 (75%) | 236/301 (78%) |

7.1.4 Statistically unusual chemical shifts [i](#)

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

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 221 | LYS | HB2 | -0.27 | 0.58 – 2.97 | -8.6 |
| 1 | A | 8 | ILE | CG1 | 13.48 | 19.24 – 36.26 | -8.4 |
| 1 | A | 199 | LYS | CG | 34.11 | 19.35 – 30.45 | 8.3 |

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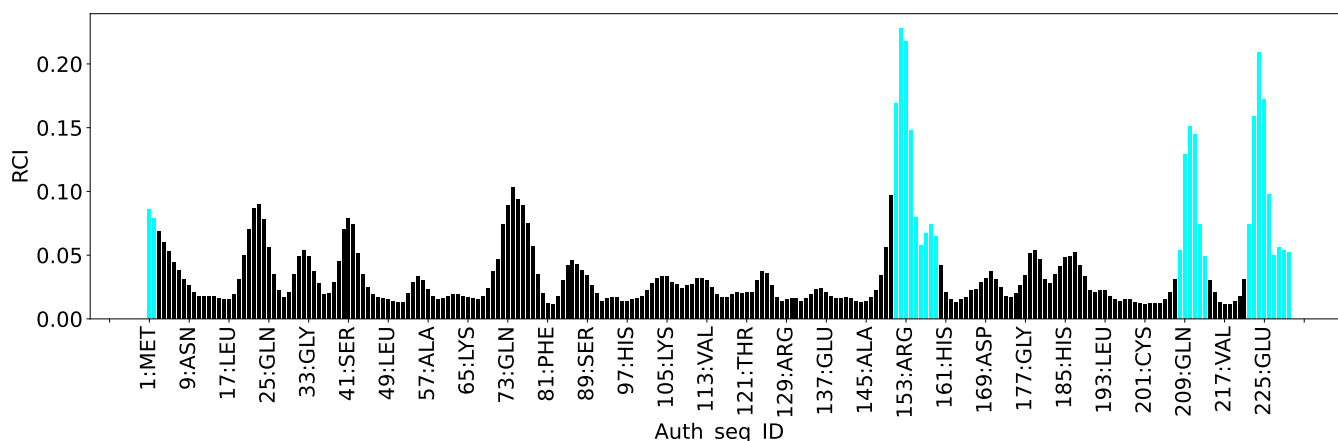
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| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 67 | ILE | CG1 | 14.15 | 19.24 – 36.26 | -8.0 |
| 1 | A | 82 | MET | H | 11.98 | 5.39 – 11.10 | 6.5 |
| 1 | A | 221 | LYS | HG2 | -0.04 | 0.13 – 2.61 | -5.7 |

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

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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 | 2462 |
| Number of shifts mapped to atoms | 2202 |
| Number of unparsed shifts | 0 |

| | |
|---|-----|
| Number of shifts with mapping errors | 260 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 6 |

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

- No matching atom found in the structure. All 260 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 2 | GLN | HB3 | 2.066 | 0.020 | 2 |
| 2 | A | 2 | GLN | HG3 | 2.309 | 0.020 | 2 |
| 2 | A | 3 | LEU | HB3 | 1.353 | 0.020 | 2 |
| 2 | A | 5 | PRO | HB3 | 1.86 | 0.020 | 2 |
| 2 | A | 6 | MET | HB3 | 1.958 | 0.020 | 2 |
| 2 | A | 6 | MET | HG3 | 2.324 | 0.020 | 2 |
| 2 | A | 7 | GLU | HB3 | 1.774 | 0.020 | 2 |
| 2 | A | 7 | GLU | HG3 | 2.143 | 0.020 | 2 |
| 2 | A | 8 | ILE | HG13 | 0.324 | 0.020 | 2 |
| 2 | A | 9 | ASN | HB3 | 2.816 | 0.020 | 2 |
| 2 | A | 10 | PRO | HB3 | 2.233 | 0.020 | 1 |
| 2 | A | 11 | GLU | HB3 | 1.992 | 0.020 | 2 |
| 2 | A | 11 | GLU | HG3 | 2.226 | 0.020 | 2 |
| 2 | A | 13 | LEU | HB3 | 1.286 | 0.020 | 2 |
| 2 | A | 14 | ASN | HB3 | 2.788 | 0.020 | 2 |
| 2 | A | 15 | LYS | HB3 | 1.85 | 0.020 | 2 |
| 2 | A | 15 | LYS | HD3 | 1.685 | 0.020 | 2 |
| 2 | A | 15 | LYS | HE3 | 2.995 | 0.020 | 2 |
| 2 | A | 15 | LYS | HG3 | 1.521 | 0.020 | 2 |
| 2 | A | 17 | LEU | HB3 | 2.086 | 0.020 | 2 |
| 2 | A | 18 | TYR | HB3 | 3.247 | 0.020 | 2 |
| 2 | A | 19 | ARG | HB3 | 1.937 | 0.020 | 2 |
| 2 | A | 19 | ARG | HD3 | 3.26 | 0.020 | 2 |
| 2 | A | 19 | ARG | HG3 | 1.883 | 0.020 | 2 |
| 2 | A | 20 | LEU | HB3 | 1.934 | 0.020 | 2 |
| 2 | A | 21 | GLY | HA3 | 4.037 | 0.020 | 2 |
| 2 | A | 24 | GLY | HA3 | 4.12 | 0.020 | 2 |
| 2 | A | 25 | GLN | HB3 | 2.101 | 0.020 | 1 |
| 2 | A | 25 | GLN | HG3 | 2.292 | 0.020 | 2 |
| 2 | A | 26 | TRP | HB3 | 2.645 | 0.020 | 2 |
| 2 | A | 27 | ARG | HB3 | 1.83 | 0.020 | 2 |
| 2 | A | 27 | ARG | HD3 | 3.158 | 0.020 | 2 |
| 2 | A | 27 | ARG | HG3 | 1.59 | 0.020 | 1 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 28 | PHE | HB3 | 3.002 | 0.020 | 2 |
| 2 | A | 30 | ASP | HB3 | 2.551 | 0.020 | 2 |
| 2 | A | 32 | LEU | HB3 | 1.665 | 0.020 | 2 |
| 2 | A | 33 | GLY | HA3 | 4.093 | 0.020 | 2 |
| 2 | A | 34 | LEU | HB3 | 1.523 | 0.020 | 2 |
| 2 | A | 35 | GLU | HB3 | 2.224 | 0.020 | 1 |
| 2 | A | 35 | GLU | HG3 | 2.334 | 0.020 | 2 |
| 2 | A | 36 | GLU | HB3 | 1.998 | 0.020 | 2 |
| 2 | A | 36 | GLU | HG3 | 2.265 | 0.020 | 2 |
| 2 | A | 37 | GLU | HB3 | 2.038 | 0.020 | 2 |
| 2 | A | 37 | GLU | HG3 | 2.294 | 0.020 | 2 |
| 2 | A | 38 | SER | HB3 | 3.791 | 0.020 | 2 |
| 2 | A | 39 | LEU | HB3 | 1.755 | 0.020 | 1 |
| 2 | A | 40 | GLY | HA3 | 4.091 | 0.020 | 2 |
| 2 | A | 41 | SER | HB3 | 3.996 | 0.020 | 2 |
| 2 | A | 43 | PRO | HB3 | 2.275 | 0.020 | 2 |
| 2 | A | 43 | PRO | HG3 | 2.025 | 0.020 | 2 |
| 2 | A | 45 | PRO | HB3 | 2.503 | 0.020 | 1 |
| 2 | A | 45 | PRO | HG3 | 2.02 | 0.020 | 1 |
| 2 | A | 47 | CYS | HB3 | 3.233 | 0.020 | 2 |
| 2 | A | 49 | LEU | HB3 | 1.64 | 0.020 | 2 |
| 2 | A | 50 | LEU | HB3 | 3.097 | 0.020 | 2 |
| 2 | A | 52 | LEU | HB3 | 2.305 | 0.020 | 2 |
| 2 | A | 53 | PHE | HB3 | 2.948 | 0.020 | 2 |
| 2 | A | 55 | LEU | HB3 | 1.564 | 0.020 | 2 |
| 2 | A | 58 | GLN | HB3 | 2.433 | 0.020 | 2 |
| 2 | A | 58 | GLN | HG3 | 2.707 | 0.020 | 2 |
| 2 | A | 59 | HIS | HB3 | 3.536 | 0.020 | 2 |
| 2 | A | 60 | GLU | HB3 | 2.118 | 0.020 | 2 |
| 2 | A | 60 | GLU | HG3 | 2.414 | 0.020 | 2 |
| 2 | A | 61 | ASN | HB3 | 2.918 | 0.020 | 2 |
| 2 | A | 62 | PHE | HB3 | 3.252 | 0.020 | 2 |
| 2 | A | 64 | LYS | HB3 | 1.926 | 0.020 | 2 |
| 2 | A | 64 | LYS | HD3 | 1.703 | 0.020 | 2 |
| 2 | A | 64 | LYS | HE3 | 2.968 | 0.020 | 2 |
| 2 | A | 64 | LYS | HG3 | 1.415 | 0.020 | 2 |
| 2 | A | 65 | LYS | HB3 | 1.883 | 0.020 | 2 |
| 2 | A | 65 | LYS | HD3 | 1.672 | 0.020 | 2 |
| 2 | A | 65 | LYS | HE3 | 2.961 | 0.020 | 2 |
| 2 | A | 65 | LYS | HG3 | 1.338 | 0.020 | 2 |
| 2 | A | 67 | ILE | HG13 | 0.83 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 68 | GLU | HB3 | 2.117 | 0.020 | 2 |
| 2 | A | 68 | GLU | HG3 | 2.405 | 0.020 | 2 |
| 2 | A | 69 | GLU | HB3 | 2.131 | 0.020 | 2 |
| 2 | A | 70 | LEU | HB3 | 1.765 | 0.020 | 2 |
| 2 | A | 71 | LYS | HB3 | 1.913 | 0.020 | 2 |
| 2 | A | 71 | LYS | HD3 | 1.738 | 0.020 | 2 |
| 2 | A | 71 | LYS | HE3 | 3.004 | 0.020 | 2 |
| 2 | A | 71 | LYS | HG3 | 1.495 | 0.020 | 2 |
| 2 | A | 72 | GLY | HA3 | 3.898 | 0.020 | 2 |
| 2 | A | 73 | GLN | HB3 | 2.036 | 0.020 | 2 |
| 2 | A | 73 | GLN | HG3 | 2.284 | 0.020 | 2 |
| 2 | A | 74 | GLU | HB3 | 1.824 | 0.020 | 2 |
| 2 | A | 74 | GLU | HG3 | 2.003 | 0.020 | 2 |
| 2 | A | 76 | SER | HB3 | 4.377 | 0.020 | 2 |
| 2 | A | 77 | PRO | HB3 | 2.361 | 0.020 | 1 |
| 2 | A | 77 | PRO | HD3 | 3.948 | 0.020 | 2 |
| 2 | A | 77 | PRO | HG3 | 2.072 | 0.020 | 2 |
| 2 | A | 78 | LYS | HB3 | 1.81 | 0.020 | 2 |
| 2 | A | 78 | LYS | HD3 | 1.663 | 0.020 | 2 |
| 2 | A | 78 | LYS | HE3 | 2.959 | 0.020 | 2 |
| 2 | A | 78 | LYS | HG3 | 1.387 | 0.020 | 2 |
| 2 | A | 80 | TYR | HB3 | 2.822 | 0.020 | 2 |
| 2 | A | 81 | PHE | HB3 | 3.389 | 0.020 | 2 |
| 2 | A | 82 | MET | HB3 | 1.818 | 0.020 | 1 |
| 2 | A | 82 | MET | HG3 | 2.34 | 0.020 | 2 |
| 2 | A | 83 | LYS | HB3 | 1.284 | 0.020 | 2 |
| 2 | A | 83 | LYS | HE3 | 3.043 | 0.020 | 2 |
| 2 | A | 86 | ILE | HG13 | 1.593 | 0.020 | 2 |
| 2 | A | 87 | GLY | HA3 | 4.069 | 0.020 | 2 |
| 2 | A | 88 | ASN | HB3 | 2.955 | 0.020 | 2 |
| 2 | A | 89 | SER | HB3 | 4.026 | 0.020 | 2 |
| 2 | A | 90 | CYS | HB3 | 2.906 | 0.020 | 2 |
| 2 | A | 91 | GLY | HA3 | 3.893 | 0.020 | 2 |
| 2 | A | 93 | ILE | HG13 | 1.122 | 0.020 | 2 |
| 2 | A | 94 | GLY | HA3 | 3.965 | 0.020 | 2 |
| 2 | A | 96 | ILE | HG13 | 2.001 | 0.020 | 2 |
| 2 | A | 97 | HIS | HB3 | 3.0 | 0.020 | 2 |
| 2 | A | 101 | ASN | HB3 | 2.911 | 0.020 | 1 |
| 2 | A | 102 | ASN | HB3 | 2.589 | 0.020 | 1 |
| 2 | A | 103 | GLN | HB3 | 2.408 | 0.020 | 2 |
| 2 | A | 103 | GLN | HG3 | 2.58 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 104 | ASP | HB3 | 2.738 | 0.020 | 2 |
| 2 | A | 105 | LYS | HB3 | 1.518 | 0.020 | 1 |
| 2 | A | 105 | LYS | HD3 | 1.667 | 0.020 | 2 |
| 2 | A | 105 | LYS | HE3 | 3.147 | 0.020 | 2 |
| 2 | A | 105 | LYS | HG3 | 1.267 | 0.020 | 2 |
| 2 | A | 106 | LEU | HB3 | 1.041 | 0.020 | 2 |
| 2 | A | 107 | GLY | HA3 | 4.365 | 0.020 | 1 |
| 2 | A | 108 | PHE | HB3 | 2.796 | 0.020 | 2 |
| 2 | A | 109 | GLU | HB3 | 2.125 | 0.020 | 2 |
| 2 | A | 109 | GLU | HG3 | 2.389 | 0.020 | 2 |
| 2 | A | 110 | ASP | HB3 | 2.625 | 0.020 | 2 |
| 2 | A | 111 | GLY | HA3 | 3.811 | 0.020 | 2 |
| 2 | A | 112 | SER | HB3 | 3.867 | 0.020 | 2 |
| 2 | A | 114 | LEU | HB3 | 1.602 | 0.020 | 2 |
| 2 | A | 115 | LYS | HB3 | 1.612 | 0.020 | 2 |
| 2 | A | 115 | LYS | HD3 | 1.299 | 0.020 | 2 |
| 2 | A | 115 | LYS | HE3 | 2.771 | 0.020 | 2 |
| 2 | A | 115 | LYS | HG3 | 1.129 | 0.020 | 2 |
| 2 | A | 116 | GLN | HB3 | 2.142 | 0.020 | 2 |
| 2 | A | 116 | GLN | HG3 | 2.463 | 0.020 | 2 |
| 2 | A | 117 | PHE | HB3 | 3.29 | 0.020 | 1 |
| 2 | A | 118 | LEU | HB3 | 1.74 | 0.020 | 2 |
| 2 | A | 119 | SER | HB3 | 3.946 | 0.020 | 2 |
| 2 | A | 120 | GLU | HB3 | 2.086 | 0.020 | 2 |
| 2 | A | 120 | GLU | HG3 | 2.208 | 0.020 | 2 |
| 2 | A | 122 | GLU | HB3 | 2.46 | 0.020 | 1 |
| 2 | A | 122 | GLU | HG3 | 2.233 | 0.020 | 2 |
| 2 | A | 123 | LYS | HB3 | 2.066 | 0.020 | 2 |
| 2 | A | 123 | LYS | HD3 | 1.675 | 0.020 | 2 |
| 2 | A | 123 | LYS | HE3 | 2.964 | 0.020 | 2 |
| 2 | A | 123 | LYS | HG3 | 1.366 | 0.020 | 2 |
| 2 | A | 124 | MET | HB3 | 2.018 | 0.020 | 2 |
| 2 | A | 124 | MET | HG3 | 2.718 | 0.020 | 2 |
| 2 | A | 125 | SER | HB3 | 4.148 | 0.020 | 2 |
| 2 | A | 126 | PRO | HB3 | 1.948 | 0.020 | 2 |
| 2 | A | 127 | GLU | HB3 | 1.954 | 0.020 | 2 |
| 2 | A | 127 | GLU | HG3 | 2.464 | 0.020 | 2 |
| 2 | A | 128 | ASP | HB3 | 2.856 | 0.020 | 2 |
| 2 | A | 129 | ARG | HB3 | 1.915 | 0.020 | 2 |
| 2 | A | 129 | ARG | HD3 | 3.037 | 0.020 | 2 |
| 2 | A | 129 | ARG | HG3 | 1.724 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 131 | LYS | HB3 | 1.984 | 0.020 | 2 |
| 2 | A | 131 | LYS | HE3 | 2.962 | 0.020 | 2 |
| 2 | A | 132 | CYS | HB3 | 3.089 | 0.020 | 1 |
| 2 | A | 133 | PHE | HB3 | 3.507 | 0.020 | 1 |
| 2 | A | 134 | GLU | HB3 | 2.221 | 0.020 | 2 |
| 2 | A | 134 | GLU | HG3 | 2.643 | 0.020 | 2 |
| 2 | A | 135 | LYS | HB3 | 2.055 | 0.020 | 2 |
| 2 | A | 135 | LYS | HD3 | 1.686 | 0.020 | 2 |
| 2 | A | 135 | LYS | HE3 | 2.982 | 0.020 | 2 |
| 2 | A | 135 | LYS | HG3 | 1.574 | 0.020 | 2 |
| 2 | A | 136 | ASN | HB3 | 2.901 | 0.020 | 2 |
| 2 | A | 137 | GLU | HB3 | 1.98 | 0.020 | 2 |
| 2 | A | 137 | GLU | HG3 | 2.34 | 0.020 | 2 |
| 2 | A | 139 | ILE | HG13 | 1.555 | 0.020 | 2 |
| 2 | A | 140 | GLN | HB3 | 2.002 | 0.020 | 2 |
| 2 | A | 140 | GLN | HG3 | 2.289 | 0.020 | 2 |
| 2 | A | 143 | HIS | HB3 | 3.476 | 0.020 | 2 |
| 2 | A | 148 | GLN | HB3 | 2.194 | 0.020 | 2 |
| 2 | A | 148 | GLN | HG3 | 2.54 | 0.020 | 2 |
| 2 | A | 149 | GLU | HB3 | 2.136 | 0.020 | 2 |
| 2 | A | 149 | GLU | HG3 | 2.577 | 0.020 | 2 |
| 2 | A | 150 | GLY | HA3 | 4.31 | 0.020 | 2 |
| 2 | A | 151 | GLN | HB3 | 1.99 | 0.020 | 2 |
| 2 | A | 151 | GLN | HG3 | 2.315 | 0.020 | 2 |
| 2 | A | 152 | CYS | HB3 | 2.807 | 0.020 | 2 |
| 2 | A | 153 | ARG | HB3 | 1.779 | 0.020 | 2 |
| 2 | A | 153 | ARG | HD3 | 3.177 | 0.020 | 2 |
| 2 | A | 153 | ARG | HG3 | 1.593 | 0.020 | 2 |
| 2 | A | 155 | ASP | HB3 | 2.831 | 0.020 | 2 |
| 2 | A | 156 | ASP | HB3 | 2.723 | 0.020 | 2 |
| 2 | A | 157 | LYS | HB3 | 1.809 | 0.020 | 2 |
| 2 | A | 157 | LYS | HD3 | 1.599 | 0.020 | 2 |
| 2 | A | 157 | LYS | HE3 | 2.95 | 0.020 | 2 |
| 2 | A | 157 | LYS | HG3 | 1.364 | 0.020 | 2 |
| 2 | A | 160 | PHE | HB3 | 2.796 | 0.020 | 2 |
| 2 | A | 161 | HIS | HB3 | 2.511 | 0.020 | 2 |
| 2 | A | 163 | ILE | HG13 | 1.196 | 0.020 | 2 |
| 2 | A | 165 | PHE | HB3 | 2.821 | 0.020 | 2 |
| 2 | A | 166 | ASN | HB3 | 2.853 | 0.020 | 2 |
| 2 | A | 167 | ASN | HB3 | 2.701 | 0.020 | 2 |
| 2 | A | 169 | ASP | HB3 | 3.312 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 170 | GLY | HA3 | 4.115 | 0.020 | 1 |
| 2 | A | 171 | HIS | HB3 | 2.973 | 0.020 | 2 |
| 2 | A | 173 | TYR | HB3 | 2.806 | 0.020 | 1 |
| 2 | A | 174 | GLU | HB3 | 2.173 | 0.020 | 2 |
| 2 | A | 175 | LEU | HB3 | 1.537 | 0.020 | 2 |
| 2 | A | 176 | ASP | HB3 | 2.765 | 0.020 | 2 |
| 2 | A | 177 | GLY | HA3 | 3.961 | 0.020 | 2 |
| 2 | A | 180 | PRO | HB3 | 2.129 | 0.020 | 2 |
| 2 | A | 181 | PHE | HB3 | 3.303 | 0.020 | 2 |
| 2 | A | 182 | PRO | HB3 | 1.873 | 0.020 | 2 |
| 2 | A | 182 | PRO | HG3 | 1.595 | 0.020 | 2 |
| 2 | A | 184 | ASN | HB3 | 3.089 | 0.020 | 2 |
| 2 | A | 185 | HIS | HB3 | 3.593 | 0.020 | 2 |
| 2 | A | 186 | GLY | HA3 | 4.552 | 0.020 | 2 |
| 2 | A | 188 | SER | HB3 | 3.737 | 0.020 | 2 |
| 2 | A | 189 | SER | HB3 | 4.06 | 0.020 | 2 |
| 2 | A | 190 | GLU | HB3 | 2.151 | 0.020 | 2 |
| 2 | A | 190 | GLU | HG3 | 2.415 | 0.020 | 2 |
| 2 | A | 191 | ASP | HB3 | 2.717 | 0.020 | 2 |
| 2 | A | 193 | LEU | HB3 | 1.734 | 0.020 | 2 |
| 2 | A | 194 | LEU | HB3 | 1.766 | 0.020 | 1 |
| 2 | A | 195 | LYS | HB3 | 1.752 | 0.020 | 2 |
| 2 | A | 195 | LYS | HD3 | 1.638 | 0.020 | 2 |
| 2 | A | 195 | LYS | HE3 | 2.935 | 0.020 | 2 |
| 2 | A | 195 | LYS | HG3 | 1.352 | 0.020 | 2 |
| 2 | A | 196 | ASP | HB3 | 2.644 | 0.020 | 2 |
| 2 | A | 199 | LYS | HB3 | 1.913 | 0.020 | 2 |
| 2 | A | 199 | LYS | HD3 | 1.661 | 0.020 | 2 |
| 2 | A | 199 | LYS | HE3 | 2.99 | 0.020 | 2 |
| 2 | A | 199 | LYS | HG3 | 2.011 | 0.020 | 2 |
| 2 | A | 201 | CYS | HB3 | 3.06 | 0.020 | 2 |
| 2 | A | 203 | GLU | HB3 | 2.451 | 0.020 | 2 |
| 2 | A | 203 | GLU | HG3 | 2.59 | 0.020 | 2 |
| 2 | A | 204 | PHE | HB3 | 3.521 | 0.020 | 2 |
| 2 | A | 206 | GLU | HB3 | 2.008 | 0.020 | 2 |
| 2 | A | 206 | GLU | HG3 | 2.326 | 0.020 | 2 |
| 2 | A | 207 | ARG | HB3 | 2.049 | 0.020 | 2 |
| 2 | A | 207 | ARG | HD3 | 3.157 | 0.020 | 2 |
| 2 | A | 207 | ARG | HG3 | 1.819 | 0.020 | 2 |
| 2 | A | 208 | GLU | HB3 | 2.412 | 0.020 | 2 |
| 2 | A | 208 | GLU | HG3 | 2.443 | 0.020 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 209 | GLN | HB3 | 2.205 | 0.020 | 2 |
| 2 | A | 209 | GLN | HG3 | 2.409 | 0.020 | 2 |
| 2 | A | 210 | GLY | HA3 | 4.05 | 0.020 | 2 |
| 2 | A | 211 | GLU | HB3 | 2.261 | 0.020 | 1 |
| 2 | A | 211 | GLU | HG3 | 2.174 | 0.020 | 2 |
| 2 | A | 213 | ARG | HB3 | 1.891 | 0.020 | 2 |
| 2 | A | 213 | ARG | HD3 | 3.225 | 0.020 | 2 |
| 2 | A | 213 | ARG | HG3 | 1.718 | 0.020 | 2 |
| 2 | A | 214 | PHE | HB3 | 3.093 | 0.020 | 2 |
| 2 | A | 215 | SER | HB3 | 3.919 | 0.020 | 2 |
| 2 | A | 219 | LEU | HB3 | 0.768 | 0.020 | 2 |
| 2 | A | 220 | CYS | HB3 | 2.797 | 0.020 | 2 |
| 2 | A | 221 | LYS | HB3 | 1.05 | 0.020 | 1 |
| 2 | A | 221 | LYS | HD3 | 1.188 | 0.020 | 2 |
| 2 | A | 221 | LYS | HE3 | 2.662 | 0.020 | 2 |
| 2 | A | 221 | LYS | HG3 | 0.568 | 0.020 | 2 |
| 2 | A | 224 | LEU | HB3 | 1.501 | 0.020 | 2 |
| 2 | A | 225 | GLU | HB3 | 1.837 | 0.020 | 2 |
| 2 | A | 225 | GLU | HG3 | 2.14 | 0.020 | 2 |
| 2 | A | 226 | HIS | HB3 | 3.041 | 0.020 | 2 |
| 2 | A | 229 | HIS | HB3 | 3.099 | 0.020 | 2 |
| 2 | A | 230 | HIS | HB3 | 3.118 | 0.020 | 2 |

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 229 | -0.18 ± 0.06 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 208 | 0.14 ± 0.14 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 228 | -0.07 ± 0.09 | None needed (< 0.5 ppm) |
| ^{15}N | 217 | 0.05 ± 0.18 | None needed (< 0.5 ppm) |

7.2.3 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 79%, i.e. 2224 atoms were assigned a chemical shift out of a possible 2803. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 1018/1031 (99%) | 410/419 (98%) | 412/414 (100%) | 196/198 (99%) |
| Sidechain | 1204/1561 (77%) | 842/1013 (83%) | 347/492 (71%) | 15/56 (27%) |
| Aromatic | 2/211 (1%) | 1/107 (1%) | 0/97 (0%) | 1/7 (14%) |
| Overall | 2224/2803 (79%) | 1253/1539 (81%) | 759/1003 (76%) | 212/261 (81%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2462 atoms were assigned a chemical shift out of a possible 3142. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 1127/1152 (98%) | 453/468 (97%) | 457/462 (99%) | 217/222 (98%) |
| Sidechain | 1333/1737 (77%) | 930/1125 (83%) | 385/546 (71%) | 18/66 (27%) |
| Aromatic | 2/253 (1%) | 1/131 (1%) | 0/109 (0%) | 1/13 (8%) |
| Overall | 2462/3142 (78%) | 1384/1724 (80%) | 842/1117 (75%) | 236/301 (78%) |

7.2.4 Statistically unusual chemical shifts [i](#)

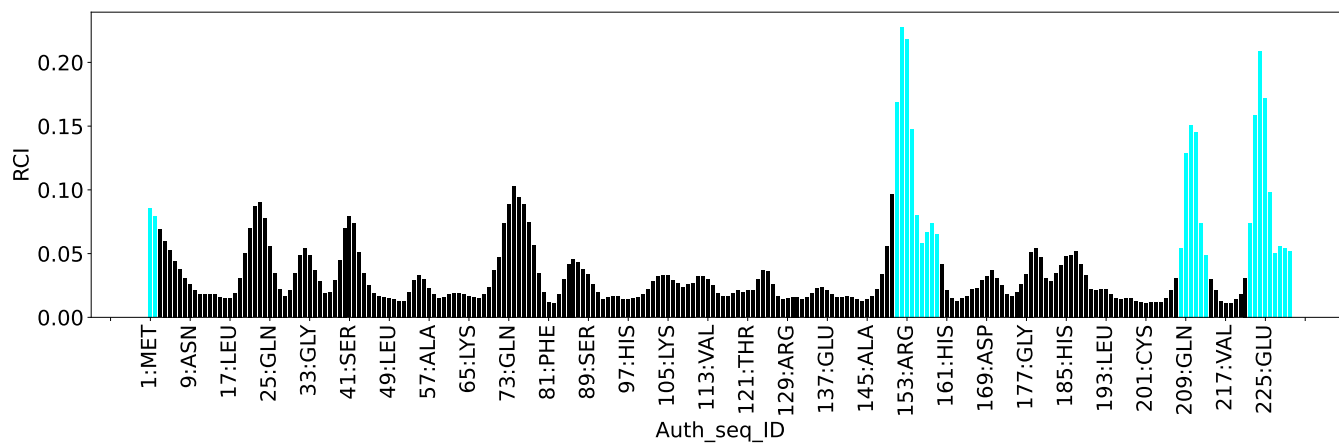
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 2 | A | 221 | LYS | HB2 | -0.27 | 0.58 – 2.97 | -8.6 |
| 2 | A | 8 | ILE | CG1 | 13.48 | 19.24 – 36.26 | -8.4 |
| 2 | A | 199 | LYS | CG | 34.11 | 19.35 – 30.45 | 8.3 |
| 2 | A | 67 | ILE | CG1 | 14.15 | 19.24 – 36.26 | -8.0 |
| 2 | A | 82 | MET | H | 11.98 | 5.39 – 11.10 | 6.5 |
| 2 | A | 221 | LYS | HG2 | -0.04 | 0.13 – 2.61 | -5.7 |

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 2375 |
| Intra-residue ($ i-j =0$) | 578 |
| Sequential ($ i-j =1$) | 724 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 475 |
| Long range ($ i-j \geq 5$) | 598 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 733 |
| Number of unmapped restraints | 4 |
| Number of restraints per residue | 13.5 |
| Number of long range restraints per residue ¹ | 2.6 |

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) | 62.7 | 0.2 |
| 0.2-0.5 (Medium) | 78.2 | 0.5 |
| >0.5 (Large) | 32.1 | 4.28 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 2.1 | 9.9 |
| 10.0-20.0 (Medium) | 0.4 | 17.55 |
| >20.0 (Large) | 0.3 | 34.04 |

9 Distance violation analysis [i](#)

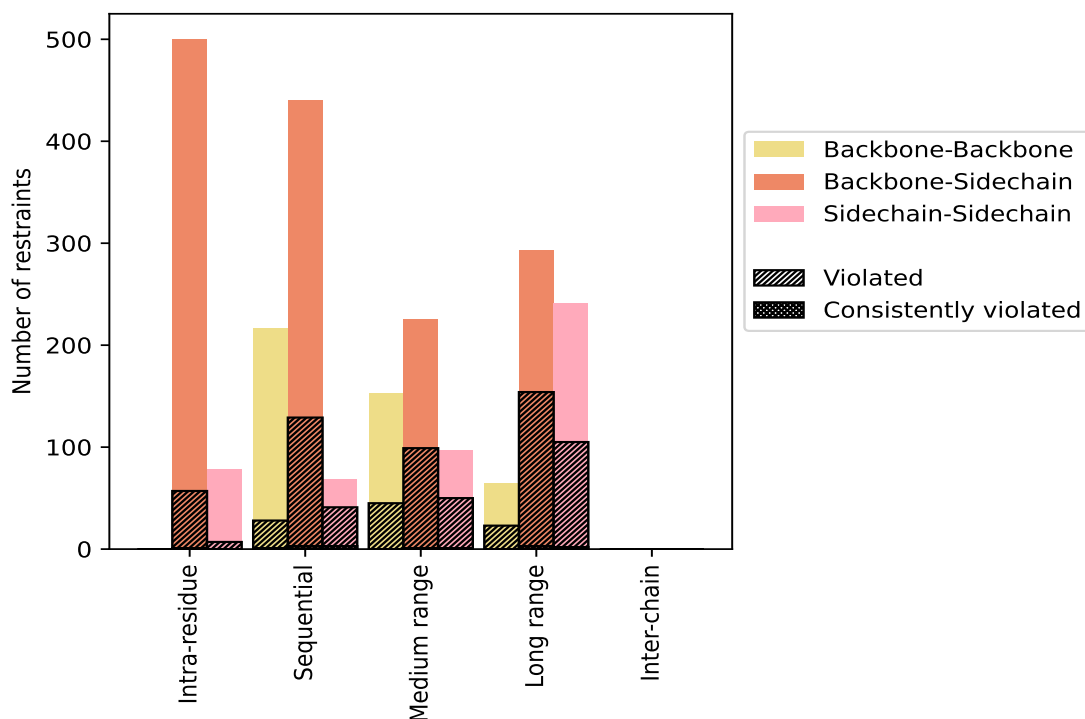
9.1 Summary of distance violations [i](#)

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 578 | 24.3 | 64 | 11.1 | 2.7 | 1 | 0.2 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 500 | 21.1 | 57 | 11.4 | 2.4 | 1 | 0.2 | 0.0 |
| Sidechain-Sidechain | 78 | 3.3 | 7 | 9.0 | 0.3 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 724 | 30.5 | 198 | 27.3 | 8.3 | 7 | 1.0 | 0.3 |
| Backbone-Backbone | 216 | 9.1 | 28 | 13.0 | 1.2 | 1 | 0.5 | 0.0 |
| Backbone-Sidechain | 440 | 18.5 | 129 | 29.3 | 5.4 | 3 | 0.7 | 0.1 |
| Sidechain-Sidechain | 68 | 2.9 | 41 | 60.3 | 1.7 | 3 | 4.4 | 0.1 |
| Medium range ($i-j >1$ & $i-j <5$) | 475 | 20.0 | 194 | 40.8 | 8.2 | 2 | 0.4 | 0.1 |
| Backbone-Backbone | 153 | 6.4 | 45 | 29.4 | 1.9 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 225 | 9.5 | 99 | 44.0 | 4.2 | 1 | 0.4 | 0.0 |
| Sidechain-Sidechain | 97 | 4.1 | 50 | 51.5 | 2.1 | 1 | 1.0 | 0.0 |
| Long range ($i-j \geq 5$) | 598 | 25.2 | 282 | 47.2 | 11.9 | 5 | 0.8 | 0.2 |
| Backbone-Backbone | 64 | 2.7 | 23 | 35.9 | 1.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 293 | 12.3 | 154 | 52.6 | 6.5 | 3 | 1.0 | 0.1 |
| Sidechain-Sidechain | 241 | 10.1 | 105 | 43.6 | 4.4 | 2 | 0.8 | 0.1 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 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 | 2375 | 100.0 | 738 | 31.1 | 31.1 | 15 | 0.6 | 0.6 |
| Backbone-Backbone | 433 | 18.2 | 96 | 22.2 | 4.0 | 1 | 0.2 | 0.0 |
| Backbone-Sidechain | 1458 | 61.4 | 439 | 30.1 | 18.5 | 8 | 0.5 | 0.3 |
| Sidechain-Sidechain | 484 | 20.4 | 203 | 41.9 | 8.5 | 6 | 1.2 | 0.3 |

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

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



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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 13 | 53 | 51 | 76 | 0 | 193 | 0.39 | 3.89 | 0.49 | 0.26 |
| 2 | 13 | 45 | 43 | 58 | 0 | 159 | 0.4 | 4.1 | 0.5 | 0.25 |
| 3 | 8 | 55 | 51 | 54 | 0 | 168 | 0.37 | 3.96 | 0.45 | 0.24 |
| 4 | 12 | 54 | 51 | 62 | 0 | 179 | 0.38 | 3.34 | 0.35 | 0.28 |
| 5 | 13 | 38 | 68 | 73 | 0 | 192 | 0.4 | 3.57 | 0.38 | 0.28 |
| 6 | 11 | 46 | 44 | 68 | 0 | 169 | 0.37 | 3.6 | 0.4 | 0.25 |
| 7 | 9 | 45 | 54 | 78 | 0 | 186 | 0.38 | 3.77 | 0.48 | 0.23 |
| 8 | 8 | 62 | 49 | 68 | 0 | 187 | 0.38 | 3.3 | 0.38 | 0.24 |
| 9 | 13 | 60 | 63 | 69 | 0 | 205 | 0.43 | 4.17 | 0.46 | 0.3 |
| 10 | 11 | 51 | 47 | 61 | 0 | 170 | 0.37 | 4.08 | 0.45 | 0.26 |

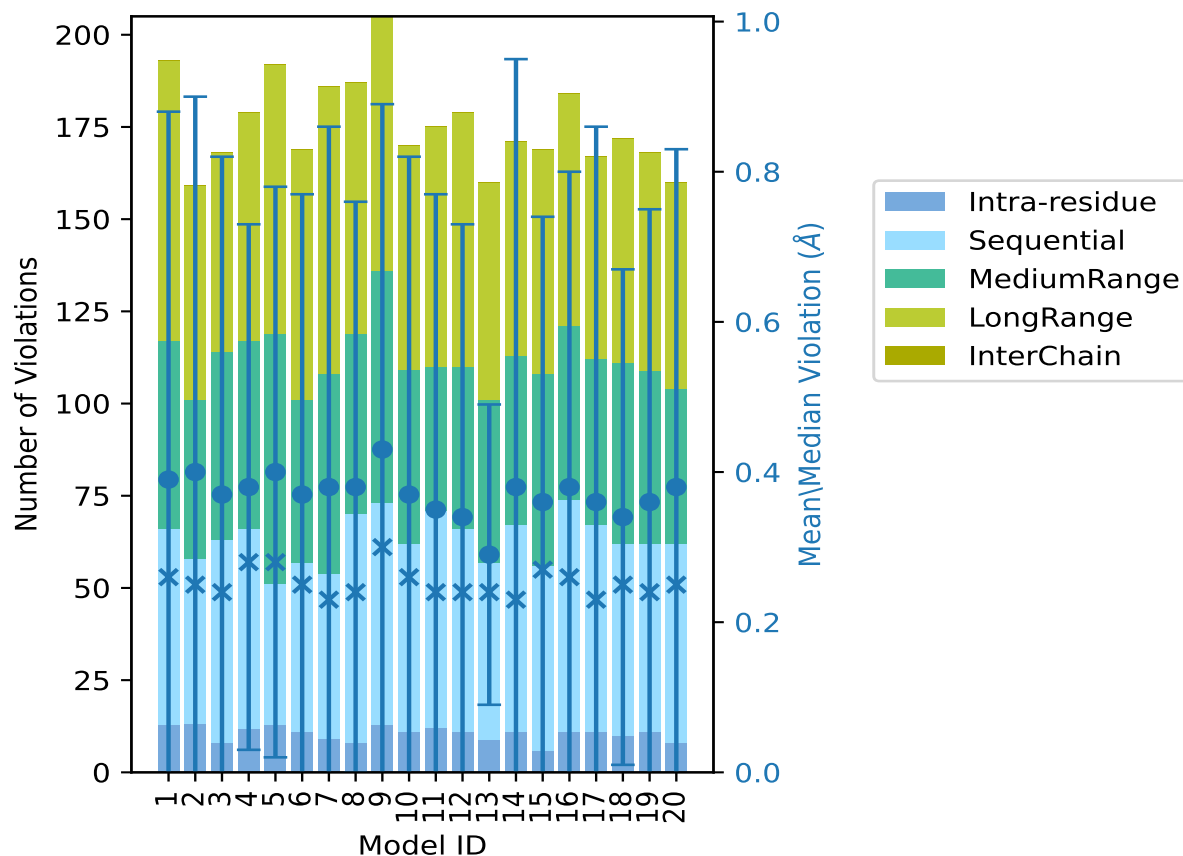
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 12 | 59 | 39 | 65 | 0 | 175 | 0.35 | 3.92 | 0.42 | 0.24 |
| 12 | 11 | 55 | 44 | 69 | 0 | 179 | 0.34 | 3.73 | 0.39 | 0.24 |
| 13 | 9 | 48 | 44 | 59 | 0 | 160 | 0.29 | 1.13 | 0.2 | 0.24 |
| 14 | 11 | 56 | 46 | 58 | 0 | 171 | 0.38 | 4.28 | 0.57 | 0.23 |
| 15 | 6 | 50 | 52 | 61 | 0 | 169 | 0.36 | 3.65 | 0.38 | 0.27 |
| 16 | 11 | 63 | 47 | 63 | 0 | 184 | 0.38 | 3.76 | 0.42 | 0.26 |
| 17 | 11 | 56 | 45 | 55 | 0 | 167 | 0.36 | 4.11 | 0.5 | 0.23 |
| 18 | 10 | 52 | 49 | 61 | 0 | 172 | 0.34 | 3.2 | 0.33 | 0.25 |
| 19 | 11 | 51 | 47 | 59 | 0 | 168 | 0.36 | 3.55 | 0.39 | 0.24 |
| 20 | 8 | 54 | 42 | 56 | 0 | 160 | 0.38 | 3.94 | 0.45 | 0.25 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

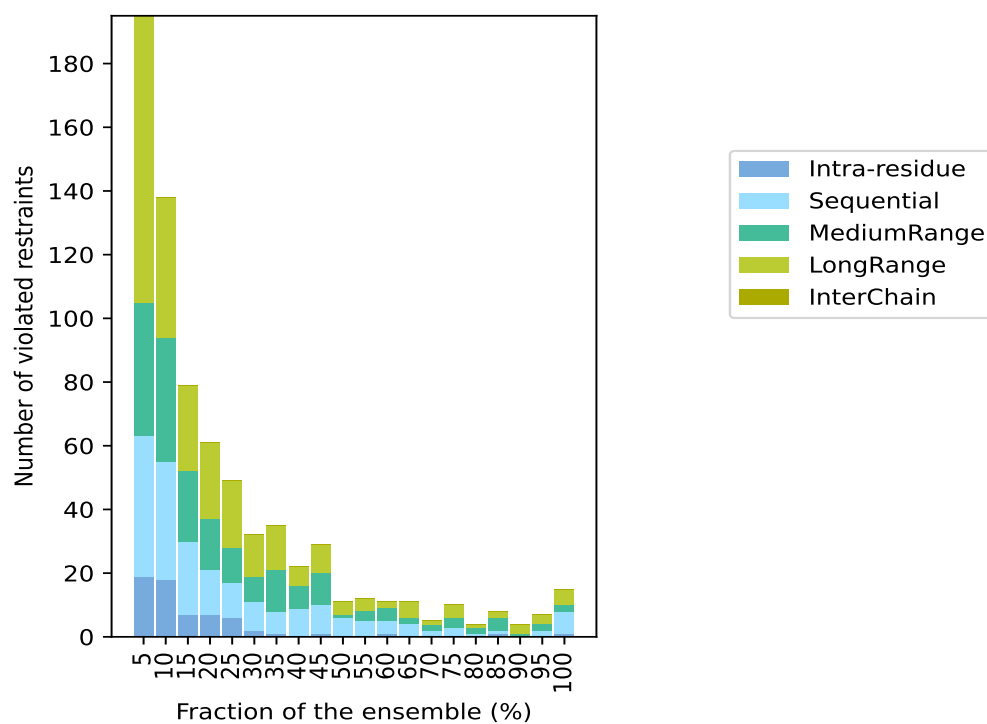
9.3 Distance violation statistics for the ensemble

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, 1637(IR:514, SQ:526, MR:281, LR:316, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 19 | 44 | 42 | 90 | 0 | 195 | 1 | 5.0 |
| 18 | 37 | 39 | 44 | 0 | 138 | 2 | 10.0 |
| 7 | 23 | 22 | 27 | 0 | 79 | 3 | 15.0 |
| 7 | 14 | 16 | 24 | 0 | 61 | 4 | 20.0 |
| 6 | 11 | 11 | 21 | 0 | 49 | 5 | 25.0 |
| 2 | 9 | 8 | 13 | 0 | 32 | 6 | 30.0 |
| 1 | 7 | 13 | 14 | 0 | 35 | 7 | 35.0 |
| 0 | 9 | 7 | 6 | 0 | 22 | 8 | 40.0 |
| 1 | 9 | 10 | 9 | 0 | 29 | 9 | 45.0 |
| 0 | 6 | 1 | 4 | 0 | 11 | 10 | 50.0 |
| 0 | 5 | 3 | 4 | 0 | 12 | 11 | 55.0 |
| 1 | 4 | 4 | 2 | 0 | 11 | 12 | 60.0 |
| 0 | 4 | 2 | 5 | 0 | 11 | 13 | 65.0 |
| 0 | 2 | 2 | 1 | 0 | 5 | 14 | 70.0 |
| 0 | 3 | 3 | 4 | 0 | 10 | 15 | 75.0 |
| 0 | 1 | 2 | 1 | 0 | 4 | 16 | 80.0 |
| 1 | 1 | 4 | 2 | 0 | 8 | 17 | 85.0 |
| 0 | 0 | 1 | 3 | 0 | 4 | 18 | 90.0 |
| 0 | 2 | 2 | 3 | 0 | 7 | 19 | 95.0 |
| 1 | 7 | 2 | 5 | 0 | 15 | 20 | 100.0 |

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

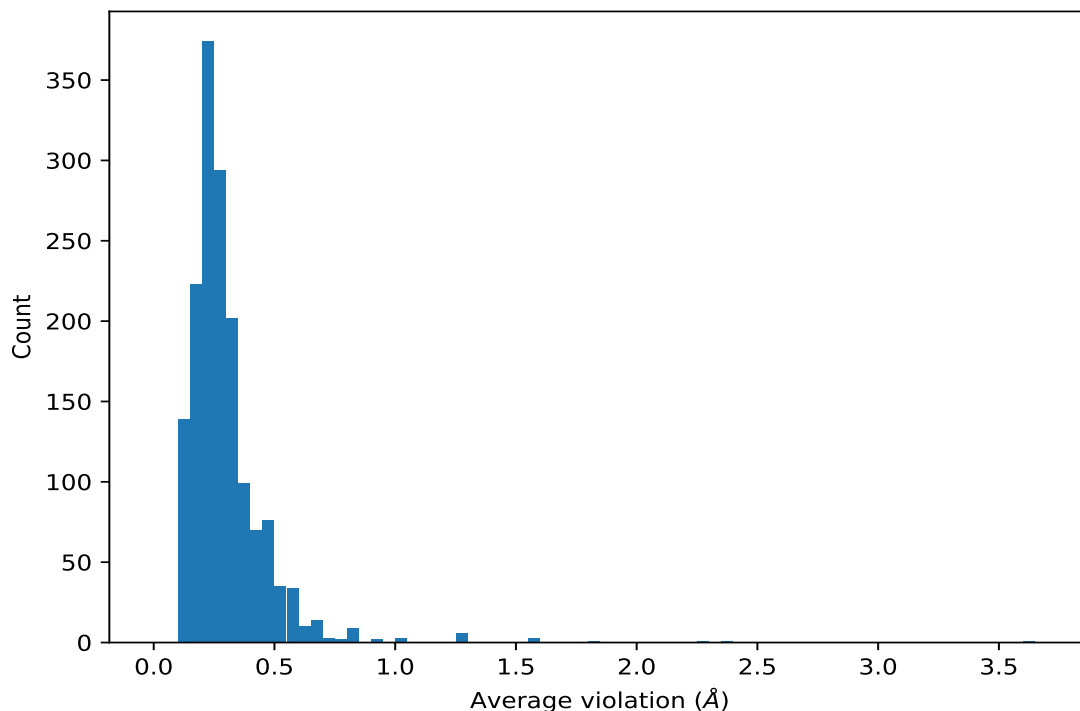
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 20 | 3.61 | 0.81 | 3.76 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 20 | 1.81 | 0.98 | 1.54 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 20 | 0.73 | 0.25 | 0.78 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 20 | 0.64 | 0.25 | 0.68 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 20 | 0.61 | 0.18 | 0.64 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 20 | 0.61 | 0.18 | 0.64 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 20 | 0.61 | 0.18 | 0.64 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 20 | 0.6 | 0.1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 20 | 0.49 | 0.2 | 0.56 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 20 | 0.49 | 0.2 | 0.56 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 20 | 0.42 | 0.11 | 0.41 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 20 | 0.34 | 0.09 | 0.34 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 20 | 0.31 | 0.03 | 0.3 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 20 | 0.26 | 0.06 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 20 | 0.25 | 0.08 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 20 | 0.25 | 0.08 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 20 | 0.24 | 0.09 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 20 | 0.24 | 0.09 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 20 | 0.24 | 0.09 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 20 | 0.24 | 0.09 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 20 | 0.24 | 0.09 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 20 | 0.24 | 0.09 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 20 | 0.2 | 0.04 | 0.2 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 20 | 0.2 | 0.04 | 0.2 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 20 | 0.2 | 0.04 | 0.2 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 19 | 2.35 | 0.52 | 2.35 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 19 | 2.26 | 0.34 | 2.26 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 19 | 0.6 | 0.19 | 0.68 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 19 | 0.6 | 0.19 | 0.68 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 19 | 0.25 | 0.08 | 0.25 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 19 | 0.25 | 0.08 | 0.25 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 19 | 0.25 | 0.08 | 0.25 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 19 | 0.21 | 0.07 | 0.22 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 19 | 0.21 | 0.05 | 0.22 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 18 | 1.58 | 0.6 | 1.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 18 | 1.58 | 0.6 | 1.48 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 18 | 1.58 | 0.6 | 1.48 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 18 | 0.51 | 0.21 | 0.55 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 18 | 0.36 | 0.15 | 0.33 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 18 | 0.36 | 0.15 | 0.33 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 18 | 0.26 | 0.11 | 0.24 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 17 | 0.52 | 0.19 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 17 | 0.52 | 0.19 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 17 | 0.52 | 0.19 | 0.47 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 17 | 0.48 | 0.23 | 0.4 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 17 | 0.48 | 0.23 | 0.4 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 17 | 0.48 | 0.23 | 0.4 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 17 | 0.47 | 0.1 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 17 | 0.47 | 0.1 | 0.49 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 17 | 0.43 | 0.17 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 17 | 0.43 | 0.17 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 17 | 0.43 | 0.17 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 17 | 0.43 | 0.17 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 17 | 0.43 | 0.17 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 17 | 0.43 | 0.17 | 0.44 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 17 | 0.32 | 0.1 | 0.32 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 17 | 0.32 | 0.14 | 0.26 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 17 | 0.31 | 0.15 | 0.26 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 17 | 0.19 | 0.07 | 0.18 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 16 | 0.35 | 0.22 | 0.3 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 16 | 0.32 | 0.16 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 16 | 0.23 | 0.06 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 16 | 0.23 | 0.06 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 16 | 0.23 | 0.06 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 16 | 0.23 | 0.06 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 16 | 0.23 | 0.06 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 16 | 0.23 | 0.06 | 0.24 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 16 | 0.2 | 0.06 | 0.2 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 15 | 1.26 | 0.58 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 15 | 1.26 | 0.58 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 15 | 1.26 | 0.58 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 15 | 1.26 | 0.58 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 15 | 1.26 | 0.58 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 15 | 1.26 | 0.58 | 1.38 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 15 | 1.03 | 0.26 | 1.14 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 15 | 1.03 | 0.26 | 1.14 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 15 | 1.03 | 0.26 | 1.14 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 15 | 0.84 | 0.11 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 15 | 0.84 | 0.11 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 15 | 0.84 | 0.11 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 15 | 0.84 | 0.11 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 15 | 0.84 | 0.11 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 15 | 0.84 | 0.11 | 0.81 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 15 | 0.54 | 0.21 | 0.55 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 15 | 0.54 | 0.21 | 0.55 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 15 | 0.54 | 0.21 | 0.55 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 15 | 0.4 | 0.21 | 0.44 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 15 | 0.38 | 0.15 | 0.36 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 15 | 0.38 | 0.15 | 0.36 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 15 | 0.35 | 0.15 | 0.36 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 15 | 0.35 | 0.18 | 0.28 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 15 | 0.18 | 0.07 | 0.16 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 15 | 0.17 | 0.04 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 15 | 0.17 | 0.04 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 15 | 0.17 | 0.04 | 0.17 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 14 | 0.67 | 0.28 | 0.64 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 14 | 0.51 | 0.27 | 0.57 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 14 | 0.51 | 0.27 | 0.57 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 14 | 0.51 | 0.27 | 0.57 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 14 | 0.51 | 0.27 | 0.57 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 14 | 0.51 | 0.27 | 0.57 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 14 | 0.51 | 0.27 | 0.57 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 14 | 0.39 | 0.21 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 14 | 0.39 | 0.21 | 0.38 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 14 | 0.39 | 0.21 | 0.38 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 14 | 0.39 | 0.24 | 0.29 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 14 | 0.22 | 0.06 | 0.2 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 13 | 0.54 | 0.21 | 0.52 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 13 | 0.54 | 0.21 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 13 | 0.53 | 0.13 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 13 | 0.53 | 0.13 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 13 | 0.53 | 0.13 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 13 | 0.53 | 0.13 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 13 | 0.53 | 0.13 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 13 | 0.53 | 0.13 | 0.52 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 13 | 0.49 | 0.23 | 0.53 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 13 | 0.48 | 0.19 | 0.51 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 13 | 0.48 | 0.19 | 0.51 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 13 | 0.48 | 0.19 | 0.51 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 13 | 0.41 | 0.21 | 0.36 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 13 | 0.41 | 0.21 | 0.36 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 13 | 0.31 | 0.11 | 0.3 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 13 | 0.31 | 0.11 | 0.3 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 13 | 0.31 | 0.11 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 13 | 0.31 | 0.18 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 13 | 0.31 | 0.18 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 13 | 0.31 | 0.18 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 13 | 0.31 | 0.18 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 13 | 0.31 | 0.18 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 13 | 0.31 | 0.18 | 0.29 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 13 | 0.26 | 0.16 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 13 | 0.26 | 0.16 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 13 | 0.26 | 0.16 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 13 | 0.26 | 0.16 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 13 | 0.26 | 0.16 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 13 | 0.26 | 0.16 | 0.19 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 13 | 0.23 | 0.1 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 13 | 0.23 | 0.1 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 13 | 0.23 | 0.1 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 13 | 0.23 | 0.1 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 13 | 0.23 | 0.1 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 13 | 0.23 | 0.1 | 0.22 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 13 | 0.17 | 0.04 | 0.16 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 13 | 0.17 | 0.04 | 0.16 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 13 | 0.17 | 0.04 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 13 | 0.16 | 0.03 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 13 | 0.16 | 0.03 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 13 | 0.16 | 0.03 | 0.15 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 12 | 0.63 | 0.2 | 0.62 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 12 | 0.63 | 0.2 | 0.62 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 12 | 0.63 | 0.2 | 0.62 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 12 | 0.63 | 0.2 | 0.62 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 12 | 0.63 | 0.2 | 0.62 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 12 | 0.63 | 0.2 | 0.62 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 12 | 0.54 | 0.5 | 0.26 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 12 | 0.36 | 0.14 | 0.34 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 12 | 0.33 | 0.15 | 0.29 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 12 | 0.33 | 0.15 | 0.29 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 12 | 0.3 | 0.18 | 0.26 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 12 | 0.3 | 0.18 | 0.26 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 12 | 0.3 | 0.18 | 0.26 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 12 | 0.25 | 0.1 | 0.24 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 12 | 0.24 | 0.11 | 0.2 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 12 | 0.17 | 0.03 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 12 | 0.17 | 0.03 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 12 | 0.17 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 12 | 0.16 | 0.03 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 12 | 0.16 | 0.03 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 12 | 0.15 | 0.02 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 12 | 0.15 | 0.02 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 12 | 0.15 | 0.02 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 12 | 0.15 | 0.02 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 12 | 0.15 | 0.02 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 12 | 0.15 | 0.02 | 0.15 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 11 | 0.53 | 0.19 | 0.5 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 11 | 0.53 | 0.19 | 0.5 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 11 | 0.5 | 0.21 | 0.52 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 11 | 0.46 | 0.21 | 0.4 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 11 | 0.44 | 0.22 | 0.41 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 11 | 0.38 | 0.17 | 0.4 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 11 | 0.38 | 0.17 | 0.4 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 11 | 0.38 | 0.17 | 0.4 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 11 | 0.3 | 0.12 | 0.28 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 11 | 0.29 | 0.1 | 0.31 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 11 | 0.23 | 0.1 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 11 | 0.23 | 0.1 | 0.21 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 11 | 0.18 | 0.05 | 0.18 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 11 | 0.17 | 0.04 | 0.17 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 11 | 0.16 | 0.06 | 0.14 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 11 | 0.15 | 0.04 | 0.14 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 10 | 0.5 | 0.21 | 0.57 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 10 | 0.5 | 0.21 | 0.57 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 10 | 0.5 | 0.21 | 0.57 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 10 | 0.37 | 0.19 | 0.39 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 10 | 0.37 | 0.19 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 10 | 0.37 | 0.19 | 0.39 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 10 | 0.37 | 0.19 | 0.39 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 10 | 0.37 | 0.19 | 0.39 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 10 | 0.37 | 0.19 | 0.39 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 10 | 0.33 | 0.2 | 0.26 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 10 | 0.33 | 0.2 | 0.26 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 10 | 0.33 | 0.2 | 0.26 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 10 | 0.33 | 0.2 | 0.26 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 10 | 0.33 | 0.2 | 0.26 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 10 | 0.33 | 0.2 | 0.26 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 10 | 0.27 | 0.13 | 0.22 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 10 | 0.27 | 0.13 | 0.22 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 10 | 0.27 | 0.13 | 0.22 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 10 | 0.25 | 0.07 | 0.24 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 10 | 0.24 | 0.1 | 0.2 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 10 | 0.24 | 0.1 | 0.2 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 10 | 0.24 | 0.1 | 0.2 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 10 | 0.23 | 0.1 | 0.22 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 10 | 0.23 | 0.1 | 0.22 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 10 | 0.23 | 0.1 | 0.22 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 10 | 0.2 | 0.07 | 0.18 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 10 | 0.19 | 0.05 | 0.2 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 10 | 0.15 | 0.03 | 0.15 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 9 | 0.65 | 0.53 | 0.24 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 9 | 0.65 | 0.53 | 0.24 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 9 | 0.57 | 0.22 | 0.6 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 9 | 0.57 | 0.22 | 0.6 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 9 | 0.57 | 0.22 | 0.6 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 9 | 0.55 | 0.4 | 0.38 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 9 | 0.43 | 0.15 | 0.4 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 9 | 0.43 | 0.15 | 0.4 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 9 | 0.43 | 0.15 | 0.4 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 9 | 0.39 | 0.17 | 0.32 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 9 | 0.36 | 0.16 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 9 | 0.36 | 0.16 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 9 | 0.36 | 0.16 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 9 | 0.36 | 0.16 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 9 | 0.36 | 0.16 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 9 | 0.36 | 0.16 | 0.35 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 9 | 0.36 | 0.15 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 9 | 0.36 | 0.15 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 9 | 0.36 | 0.15 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 9 | 0.34 | 0.17 | 0.39 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 9 | 0.33 | 0.14 | 0.3 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 9 | 0.32 | 0.11 | 0.31 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 9 | 0.31 | 0.1 | 0.31 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 9 | 0.29 | 0.15 | 0.25 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 9 | 0.28 | 0.23 | 0.23 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 9 | 0.28 | 0.1 | 0.25 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 9 | 0.28 | 0.09 | 0.28 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 9 | 0.28 | 0.09 | 0.28 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 9 | 0.28 | 0.09 | 0.28 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 9 | 0.27 | 0.15 | 0.22 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 9 | 0.27 | 0.15 | 0.22 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 9 | 0.27 | 0.15 | 0.22 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 9 | 0.27 | 0.05 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 9 | 0.27 | 0.05 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 9 | 0.27 | 0.05 | 0.27 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 9 | 0.27 | 0.13 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 9 | 0.27 | 0.13 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 9 | 0.27 | 0.13 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 9 | 0.27 | 0.13 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 9 | 0.27 | 0.13 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 9 | 0.27 | 0.13 | 0.25 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 9 | 0.25 | 0.1 | 0.24 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 9 | 0.24 | 0.1 | 0.2 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 9 | 0.21 | 0.08 | 0.22 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 9 | 0.19 | 0.05 | 0.19 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 9 | 0.19 | 0.04 | 0.19 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 9 | 0.16 | 0.05 | 0.13 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 9 | 0.13 | 0.01 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 9 | 0.12 | 0.01 | 0.12 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 9 | 0.12 | 0.01 | 0.12 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 9 | 0.12 | 0.01 | 0.12 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 9 | 0.12 | 0.02 | 0.12 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 8 | 0.77 | 0.33 | 0.71 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 8 | 0.77 | 0.33 | 0.71 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 8 | 0.48 | 0.2 | 0.55 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 8 | 0.38 | 0.23 | 0.29 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 8 | 0.38 | 0.23 | 0.29 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 8 | 0.38 | 0.23 | 0.29 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 8 | 0.38 | 0.12 | 0.36 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 8 | 0.38 | 0.12 | 0.36 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 8 | 0.38 | 0.12 | 0.36 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 8 | 0.38 | 0.12 | 0.36 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 8 | 0.38 | 0.1 | 0.38 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 8 | 0.37 | 0.11 | 0.36 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 8 | 0.37 | 0.11 | 0.36 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 8 | 0.37 | 0.11 | 0.36 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 8 | 0.37 | 0.11 | 0.36 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 8 | 0.37 | 0.11 | 0.36 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 8 | 0.37 | 0.11 | 0.36 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 8 | 0.36 | 0.16 | 0.37 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 8 | 0.33 | 0.1 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 8 | 0.3 | 0.06 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 8 | 0.3 | 0.06 | 0.32 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 8 | 0.28 | 0.13 | 0.27 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 8 | 0.27 | 0.13 | 0.22 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 8 | 0.25 | 0.1 | 0.22 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 8 | 0.24 | 0.07 | 0.24 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 8 | 0.24 | 0.07 | 0.24 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 8 | 0.24 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 8 | 0.2 | 0.07 | 0.18 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 8 | 0.2 | 0.07 | 0.18 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 8 | 0.19 | 0.04 | 0.18 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 8 | 0.19 | 0.04 | 0.18 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 8 | 0.19 | 0.04 | 0.18 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 8 | 0.19 | 0.11 | 0.15 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 8 | 0.15 | 0.07 | 0.12 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 8 | 0.14 | 0.02 | 0.14 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 8 | 0.13 | 0.04 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 8 | 0.13 | 0.04 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 8 | 0.13 | 0.04 | 0.11 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 8 | 0.12 | 0.02 | 0.12 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 7 | 0.57 | 0.28 | 0.51 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 7 | 0.55 | 0.24 | 0.52 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 7 | 0.49 | 0.24 | 0.44 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 7 | 0.49 | 0.24 | 0.44 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 7 | 0.49 | 0.24 | 0.44 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 7 | 0.49 | 0.24 | 0.44 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 7 | 0.49 | 0.24 | 0.44 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 7 | 0.49 | 0.24 | 0.44 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 7 | 0.49 | 0.24 | 0.55 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 7 | 0.45 | 0.13 | 0.42 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 7 | 0.45 | 0.13 | 0.42 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 7 | 0.45 | 0.13 | 0.42 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 7 | 0.41 | 0.16 | 0.43 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 7 | 0.4 | 0.11 | 0.38 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 7 | 0.36 | 0.15 | 0.36 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 7 | 0.35 | 0.13 | 0.39 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 7 | 0.35 | 0.13 | 0.39 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 7 | 0.35 | 0.13 | 0.39 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 7 | 0.34 | 0.17 | 0.26 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 7 | 0.34 | 0.17 | 0.26 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 7 | 0.33 | 0.22 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 7 | 0.33 | 0.22 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 7 | 0.33 | 0.22 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 7 | 0.33 | 0.22 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 7 | 0.33 | 0.22 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 7 | 0.33 | 0.22 | 0.24 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 7 | 0.32 | 0.08 | 0.33 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 7 | 0.31 | 0.16 | 0.24 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 7 | 0.31 | 0.16 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 7 | 0.31 | 0.16 | 0.24 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 7 | 0.31 | 0.16 | 0.24 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 7 | 0.31 | 0.16 | 0.24 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 7 | 0.31 | 0.16 | 0.24 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 7 | 0.3 | 0.12 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 7 | 0.3 | 0.12 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 7 | 0.3 | 0.12 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 7 | 0.3 | 0.12 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 7 | 0.3 | 0.12 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 7 | 0.3 | 0.12 | 0.28 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 7 | 0.28 | 0.06 | 0.3 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 7 | 0.28 | 0.06 | 0.3 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 7 | 0.28 | 0.06 | 0.3 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 7 | 0.28 | 0.19 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 7 | 0.28 | 0.19 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 7 | 0.28 | 0.19 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 7 | 0.28 | 0.19 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 7 | 0.28 | 0.19 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 7 | 0.28 | 0.19 | 0.22 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 7 | 0.27 | 0.12 | 0.34 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 7 | 0.26 | 0.09 | 0.26 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 7 | 0.26 | 0.09 | 0.26 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 7 | 0.26 | 0.09 | 0.26 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 7 | 0.26 | 0.12 | 0.22 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 7 | 0.25 | 0.11 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 7 | 0.25 | 0.11 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 7 | 0.25 | 0.11 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 7 | 0.25 | 0.11 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 7 | 0.25 | 0.11 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 7 | 0.25 | 0.11 | 0.25 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 7 | 0.24 | 0.13 | 0.17 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 7 | 0.24 | 0.06 | 0.28 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 7 | 0.23 | 0.14 | 0.16 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 7 | 0.23 | 0.14 | 0.16 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 7 | 0.22 | 0.05 | 0.2 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 7 | 0.22 | 0.06 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 7 | 0.21 | 0.1 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 7 | 0.21 | 0.1 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 7 | 0.21 | 0.1 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 7 | 0.21 | 0.1 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 7 | 0.21 | 0.1 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 7 | 0.21 | 0.1 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 7 | 0.21 | 0.1 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 7 | 0.21 | 0.1 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 7 | 0.21 | 0.1 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 7 | 0.21 | 0.1 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 7 | 0.21 | 0.1 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 7 | 0.21 | 0.1 | 0.16 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 7 | 0.21 | 0.08 | 0.21 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 7 | 0.2 | 0.06 | 0.21 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 7 | 0.19 | 0.06 | 0.22 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 7 | 0.19 | 0.06 | 0.21 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 7 | 0.19 | 0.06 | 0.21 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 7 | 0.17 | 0.02 | 0.16 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 7 | 0.17 | 0.02 | 0.16 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 7 | 0.16 | 0.03 | 0.14 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 7 | 0.15 | 0.04 | 0.15 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 6 | 0.84 | 0.29 | 0.86 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 6 | 0.84 | 0.29 | 0.86 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 6 | 0.55 | 0.31 | 0.45 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 6 | 0.55 | 0.31 | 0.45 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 6 | 0.45 | 0.26 | 0.38 |
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 6 | 0.45 | 0.26 | 0.38 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 6 | 0.45 | 0.26 | 0.38 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 6 | 0.35 | 0.18 | 0.27 |
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 6 | 0.35 | 0.18 | 0.27 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 6 | 0.35 | 0.18 | 0.27 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 6 | 0.34 | 0.11 | 0.32 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 6 | 0.33 | 0.18 | 0.25 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 6 | 0.32 | 0.19 | 0.3 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 6 | 0.32 | 0.19 | 0.26 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 6 | 0.31 | 0.16 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 6 | 0.31 | 0.12 | 0.26 |
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 6 | 0.31 | 0.12 | 0.26 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 6 | 0.31 | 0.12 | 0.26 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 6 | 0.31 | 0.12 | 0.26 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 6 | 0.31 | 0.12 | 0.26 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 6 | 0.31 | 0.12 | 0.26 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 6 | 0.31 | 0.12 | 0.29 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 6 | 0.3 | 0.1 | 0.26 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 6 | 0.26 | 0.09 | 0.26 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 6 | 0.26 | 0.13 | 0.24 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 6 | 0.26 | 0.13 | 0.24 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 6 | 0.26 | 0.13 | 0.24 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 6 | 0.26 | 0.07 | 0.26 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 6 | 0.26 | 0.07 | 0.26 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 6 | 0.26 | 0.07 | 0.26 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 6 | 0.25 | 0.08 | 0.26 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 6 | 0.24 | 0.07 | 0.24 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 6 | 0.24 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 6 | 0.24 | 0.07 | 0.24 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 6 | 0.24 | 0.07 | 0.24 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 6 | 0.24 | 0.07 | 0.24 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 6 | 0.24 | 0.07 | 0.24 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 6 | 0.24 | 0.04 | 0.22 |
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 6 | 0.24 | 0.04 | 0.22 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 6 | 0.24 | 0.04 | 0.22 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 6 | 0.24 | 0.04 | 0.22 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 6 | 0.24 | 0.04 | 0.22 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 6 | 0.24 | 0.04 | 0.22 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 6 | 0.22 | 0.07 | 0.18 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 6 | 0.22 | 0.07 | 0.18 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 6 | 0.22 | 0.07 | 0.18 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 6 | 0.22 | 0.07 | 0.19 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 6 | 0.22 | 0.07 | 0.19 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 6 | 0.21 | 0.05 | 0.19 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 6 | 0.21 | 0.06 | 0.2 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 6 | 0.21 | 0.08 | 0.2 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 6 | 0.2 | 0.08 | 0.16 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 6 | 0.2 | 0.08 | 0.16 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 6 | 0.2 | 0.08 | 0.16 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 6 | 0.2 | 0.08 | 0.16 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 6 | 0.2 | 0.08 | 0.16 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 6 | 0.2 | 0.08 | 0.16 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 6 | 0.18 | 0.09 | 0.14 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 6 | 0.17 | 0.04 | 0.16 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 6 | 0.16 | 0.03 | 0.15 |
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 6 | 0.13 | 0.03 | 0.12 |
| (1,1574) | 1:166:A:ASN:H | 1:175:A:LEU:HG | 5 | 0.83 | 0.12 | 0.86 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE21 | 5 | 0.73 | 0.62 | 0.35 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE22 | 5 | 0.73 | 0.62 | 0.35 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE21 | 5 | 0.68 | 0.07 | 0.68 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE22 | 5 | 0.68 | 0.07 | 0.68 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE1 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE2 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE3 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE1 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE2 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE3 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE1 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE2 | 5 | 0.56 | 0.31 | 0.59 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE3 | 5 | 0.56 | 0.31 | 0.59 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1885) | 1:25:A:GLN:HE21 | 1:26:A:TRP:H | 5 | 0.46 | 0.21 | 0.49 |
| (1,1885) | 1:25:A:GLN:HE22 | 1:26:A:TRP:H | 5 | 0.46 | 0.21 | 0.49 |
| (1,669) | 1:189:A:SER:H | 1:193:A:LEU:H | 5 | 0.43 | 0.2 | 0.44 |
| (1,2189) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 5 | 0.41 | 0.28 | 0.26 |
| (1,2189) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 5 | 0.41 | 0.28 | 0.26 |
| (1,2189) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 5 | 0.41 | 0.28 | 0.26 |
| (1,1575) | 1:175:A:LEU:HG | 1:176:A:ASP:H | 5 | 0.37 | 0.11 | 0.41 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD11 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD12 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD13 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD11 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD12 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD13 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD11 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD12 | 5 | 0.33 | 0.02 | 0.34 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD13 | 5 | 0.33 | 0.02 | 0.34 |
| (1,1085) | 1:81:A:PHE:HE1 | 1:175:A:LEU:HB2 | 5 | 0.33 | 0.14 | 0.23 |
| (1,1085) | 1:81:A:PHE:HE2 | 1:175:A:LEU:HB2 | 5 | 0.33 | 0.14 | 0.23 |
| (1,737) | 1:164:A:LEU:H | 1:177:A:GLY:H | 5 | 0.32 | 0.21 | 0.17 |
| (1,879) | 1:8:A:ILE:HG21 | 1:216:A:ALA:H | 5 | 0.32 | 0.17 | 0.36 |
| (1,879) | 1:8:A:ILE:HG22 | 1:216:A:ALA:H | 5 | 0.32 | 0.17 | 0.36 |
| (1,879) | 1:8:A:ILE:HG23 | 1:216:A:ALA:H | 5 | 0.32 | 0.17 | 0.36 |
| (1,1576) | 1:175:A:LEU:HG | 1:183:A:VAL:H | 5 | 0.32 | 0.15 | 0.25 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD11 | 5 | 0.31 | 0.12 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD12 | 5 | 0.31 | 0.12 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD13 | 5 | 0.31 | 0.12 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD11 | 5 | 0.31 | 0.12 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD12 | 5 | 0.31 | 0.12 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD13 | 5 | 0.31 | 0.12 | 0.31 |
| (1,496) | 1:53:A:PHE:HB2 | 1:215:A:SER:H | 5 | 0.3 | 0.13 | 0.25 |
| (1,1189) | 1:34:A:LEU:H | 1:38:A:SER:HB2 | 5 | 0.29 | 0.08 | 0.28 |
| (1,1763) | 1:19:A:ARG:HB2 | 1:20:A:LEU:HA | 5 | 0.29 | 0.09 | 0.25 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD1 | 5 | 0.29 | 0.14 | 0.32 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD2 | 5 | 0.29 | 0.14 | 0.32 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE1 | 5 | 0.28 | 0.08 | 0.31 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE2 | 5 | 0.28 | 0.08 | 0.31 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE3 | 5 | 0.28 | 0.08 | 0.31 |
| (1,1398) | 1:81:A:PHE:H | 1:82:A:MET:HA | 5 | 0.27 | 0.24 | 0.16 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD1 | 5 | 0.26 | 0.09 | 0.25 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD2 | 5 | 0.26 | 0.09 | 0.25 |
| (1,2031) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HA | 5 | 0.26 | 0.08 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HA | 5 | 0.26 | 0.08 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2031) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HA | 5 | 0.26 | 0.08 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HA | 5 | 0.26 | 0.08 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HA | 5 | 0.26 | 0.08 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HA | 5 | 0.26 | 0.08 | 0.26 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD21 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD22 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD21 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD22 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD21 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD22 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD21 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD22 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD21 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD22 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD21 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD22 | 5 | 0.26 | 0.19 | 0.23 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE21 | 5 | 0.26 | 0.1 | 0.28 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE22 | 5 | 0.26 | 0.1 | 0.28 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE1 | 5 | 0.26 | 0.09 | 0.25 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE2 | 5 | 0.26 | 0.09 | 0.25 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE3 | 5 | 0.26 | 0.09 | 0.25 |
| (1,358) | 1:127:A:GLU:H | 1:128:A:ASP:HB2 | 5 | 0.25 | 0.04 | 0.25 |
| (1,590) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 5 | 0.25 | 0.18 | 0.14 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG11 | 5 | 0.24 | 0.08 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG12 | 5 | 0.24 | 0.08 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG13 | 5 | 0.24 | 0.08 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG21 | 5 | 0.24 | 0.08 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG22 | 5 | 0.24 | 0.08 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG23 | 5 | 0.24 | 0.08 | 0.24 |
| (1,844) | 1:132:A:CYS:HA | 1:135:A:LYS:HE2 | 5 | 0.23 | 0.05 | 0.2 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG11 | 5 | 0.23 | 0.04 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG12 | 5 | 0.23 | 0.04 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG13 | 5 | 0.23 | 0.04 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG21 | 5 | 0.23 | 0.04 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG22 | 5 | 0.23 | 0.04 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG23 | 5 | 0.23 | 0.04 | 0.23 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD1 | 5 | 0.22 | 0.03 | 0.21 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD2 | 5 | 0.22 | 0.03 | 0.21 |
| (1,1428) | 1:23:A:ALA:HB1 | 1:107:A:GLY:HA2 | 5 | 0.22 | 0.06 | 0.19 |
| (1,1428) | 1:23:A:ALA:HB2 | 1:107:A:GLY:HA2 | 5 | 0.22 | 0.06 | 0.19 |
| (1,1428) | 1:23:A:ALA:HB3 | 1:107:A:GLY:HA2 | 5 | 0.22 | 0.06 | 0.19 |
| (1,1306) | 1:48:A:ALA:HB1 | 1:218:A:ALA:HA | 5 | 0.21 | 0.12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1306) | 1:48:A:ALA:HB2 | 1:218:A:ALA:HA | 5 | 0.21 | 0.12 | 0.16 |
| (1,1306) | 1:48:A:ALA:HB3 | 1:218:A:ALA:HA | 5 | 0.21 | 0.12 | 0.16 |
| (1,787) | 1:28:A:PHE:HA | 1:217:A:VAL:HB | 5 | 0.21 | 0.05 | 0.22 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG11 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG12 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG13 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG21 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG22 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG23 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG11 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG12 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG13 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG21 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG22 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG23 | 5 | 0.21 | 0.08 | 0.17 |
| (1,1081) | 1:27:A:ARG:H | 1:28:A:PHE:HA | 5 | 0.19 | 0.11 | 0.12 |
| (1,1233) | 1:154:A:VAL:HA | 1:156:A:ASP:HB2 | 5 | 0.19 | 0.04 | 0.18 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD11 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD12 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD13 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD21 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD22 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD23 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD11 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD12 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD13 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD21 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD22 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD23 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD11 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD12 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD13 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD21 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD22 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD23 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD11 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD12 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD13 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD21 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD22 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD23 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD11 | 5 | 0.18 | 0.05 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD12 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD13 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD21 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD22 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD23 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD11 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD12 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD13 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD21 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD22 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD23 | 5 | 0.18 | 0.05 | 0.16 |
| (1,1210) | 1:215:A:SER:HB2 | 1:216:A:ALA:H | 5 | 0.17 | 0.05 | 0.15 |
| (1,141) | 1:122:A:GLU:HA | 1:124:A:MET:H | 5 | 0.17 | 0.05 | 0.19 |
| (1,1564) | 1:74:A:GLU:HA | 1:75:A:VAL:H | 5 | 0.16 | 0.01 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD11 | 5 | 0.16 | 0.04 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD12 | 5 | 0.16 | 0.04 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD13 | 5 | 0.16 | 0.04 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD21 | 5 | 0.16 | 0.04 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD22 | 5 | 0.16 | 0.04 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD23 | 5 | 0.16 | 0.04 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB1 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB2 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB3 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB1 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB2 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB3 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB1 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB2 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB3 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB1 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB2 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB3 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB1 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB2 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB3 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB1 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB2 | 5 | 0.16 | 0.05 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB3 | 5 | 0.16 | 0.05 | 0.15 |
| (1,632) | 1:34:A:LEU:HD11 | 1:35:A:GLU:H | 5 | 0.16 | 0.06 | 0.13 |
| (1,632) | 1:34:A:LEU:HD12 | 1:35:A:GLU:H | 5 | 0.16 | 0.06 | 0.13 |
| (1,632) | 1:34:A:LEU:HD13 | 1:35:A:GLU:H | 5 | 0.16 | 0.06 | 0.13 |
| (1,632) | 1:34:A:LEU:HD21 | 1:35:A:GLU:H | 5 | 0.16 | 0.06 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,632) | 1:34:A:LEU:HD22 | 1:35:A:GLU:H | 5 | 0.16 | 0.06 | 0.13 |
| (1,632) | 1:34:A:LEU:HD23 | 1:35:A:GLU:H | 5 | 0.16 | 0.06 | 0.13 |
| (1,681) | 1:194:A:LEU:HA | 1:197:A:ALA:H | 5 | 0.16 | 0.03 | 0.16 |
| (1,512) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1577) | 1:164:A:LEU:HD11 | 1:175:A:LEU:HG | 5 | 0.15 | 0.03 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD12 | 1:175:A:LEU:HG | 5 | 0.15 | 0.03 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD13 | 1:175:A:LEU:HG | 5 | 0.15 | 0.03 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD21 | 1:175:A:LEU:HG | 5 | 0.15 | 0.03 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD22 | 1:175:A:LEU:HG | 5 | 0.15 | 0.03 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD23 | 1:175:A:LEU:HG | 5 | 0.15 | 0.03 | 0.16 |
| (1,2241) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HB2 | 5 | 0.15 | 0.04 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HB2 | 5 | 0.15 | 0.04 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HB2 | 5 | 0.15 | 0.04 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HB2 | 5 | 0.15 | 0.04 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HB2 | 5 | 0.15 | 0.04 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HB2 | 5 | 0.15 | 0.04 | 0.13 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG21 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG22 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG23 | 5 | 0.13 | 0.02 | 0.13 |
| (1,2015) | 1:61:A:ASN:HD21 | 1:62:A:PHE:H | 4 | 0.91 | 0.03 | 0.9 |
| (1,2015) | 1:61:A:ASN:HD22 | 1:62:A:PHE:H | 4 | 0.91 | 0.03 | 0.9 |
| (1,1732) | 1:122:A:GLU:HG2 | 1:123:A:LYS:HG2 | 4 | 0.58 | 0.3 | 0.57 |
| (1,1003) | 1:131:A:LYS:HA | 1:134:A:GLU:HB2 | 4 | 0.57 | 0.05 | 0.56 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE1 | 4 | 0.54 | 0.26 | 0.56 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE2 | 4 | 0.54 | 0.26 | 0.56 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE3 | 4 | 0.54 | 0.26 | 0.56 |
| (1,2) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 4 | 0.49 | 0.17 | 0.49 |
| (1,2) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 4 | 0.49 | 0.17 | 0.49 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD11 | 4 | 0.46 | 0.11 | 0.42 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD12 | 4 | 0.46 | 0.11 | 0.42 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD13 | 4 | 0.46 | 0.11 | 0.42 |
| (1,971) | 1:12:A:MET:HE1 | 1:150:A:GLY:H | 4 | 0.45 | 0.13 | 0.42 |
| (1,971) | 1:12:A:MET:HE2 | 1:150:A:GLY:H | 4 | 0.45 | 0.13 | 0.42 |
| (1,971) | 1:12:A:MET:HE3 | 1:150:A:GLY:H | 4 | 0.45 | 0.13 | 0.42 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB1 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB2 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB3 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB1 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB2 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB3 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB1 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB2 | 4 | 0.42 | 0.17 | 0.43 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB3 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB1 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB2 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB3 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB1 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB2 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB3 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB1 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB2 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB3 | 4 | 0.42 | 0.17 | 0.43 |
| (1,1717) | 1:118:A:LEU:H | 1:120:A:GLU:HG2 | 4 | 0.39 | 0.18 | 0.36 |
| (1,962) | 1:124:A:MET:HE1 | 1:129:A:ARG:H | 4 | 0.38 | 0.22 | 0.38 |
| (1,962) | 1:124:A:MET:HE2 | 1:129:A:ARG:H | 4 | 0.38 | 0.22 | 0.38 |
| (1,962) | 1:124:A:MET:HE3 | 1:129:A:ARG:H | 4 | 0.38 | 0.22 | 0.38 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE21 | 4 | 0.37 | 0.08 | 0.36 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE22 | 4 | 0.37 | 0.08 | 0.36 |
| (1,60) | 1:36:A:GLU:HB2 | 1:37:A:GLU:H | 4 | 0.37 | 0.02 | 0.37 |
| (1,1997) | 1:55:A:LEU:HD11 | 1:161:A:HIS:H | 4 | 0.36 | 0.1 | 0.38 |
| (1,1997) | 1:55:A:LEU:HD12 | 1:161:A:HIS:H | 4 | 0.36 | 0.1 | 0.38 |
| (1,1997) | 1:55:A:LEU:HD13 | 1:161:A:HIS:H | 4 | 0.36 | 0.1 | 0.38 |
| (1,1997) | 1:55:A:LEU:HD21 | 1:161:A:HIS:H | 4 | 0.36 | 0.1 | 0.38 |
| (1,1997) | 1:55:A:LEU:HD22 | 1:161:A:HIS:H | 4 | 0.36 | 0.1 | 0.38 |
| (1,1997) | 1:55:A:LEU:HD23 | 1:161:A:HIS:H | 4 | 0.36 | 0.1 | 0.38 |
| (1,1848) | 1:13:A:LEU:HA | 1:17:A:LEU:HB2 | 4 | 0.34 | 0.13 | 0.36 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE1 | 4 | 0.33 | 0.18 | 0.32 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE2 | 4 | 0.33 | 0.18 | 0.32 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE3 | 4 | 0.33 | 0.18 | 0.32 |
| (1,1676) | 1:25:A:GLN:HG2 | 1:221:A:LYS:HE2 | 4 | 0.33 | 0.09 | 0.38 |
| (1,706) | 1:73:A:GLN:HA | 1:74:A:GLU:H | 4 | 0.32 | 0.16 | 0.29 |
| (1,976) | 1:82:A:MET:HE1 | 1:93:A:ILE:H | 4 | 0.32 | 0.12 | 0.34 |
| (1,976) | 1:82:A:MET:HE2 | 1:93:A:ILE:H | 4 | 0.32 | 0.12 | 0.34 |
| (1,976) | 1:82:A:MET:HE3 | 1:93:A:ILE:H | 4 | 0.32 | 0.12 | 0.34 |
| (1,403) | 1:99:A:VAL:HG11 | 1:103:A:GLN:HE21 | 4 | 0.31 | 0.1 | 0.26 |
| (1,403) | 1:99:A:VAL:HG12 | 1:103:A:GLN:HE21 | 4 | 0.31 | 0.1 | 0.26 |
| (1,403) | 1:99:A:VAL:HG13 | 1:103:A:GLN:HE21 | 4 | 0.31 | 0.1 | 0.26 |
| (1,403) | 1:99:A:VAL:HG21 | 1:103:A:GLN:HE21 | 4 | 0.31 | 0.1 | 0.26 |
| (1,403) | 1:99:A:VAL:HG22 | 1:103:A:GLN:HE21 | 4 | 0.31 | 0.1 | 0.26 |
| (1,403) | 1:99:A:VAL:HG23 | 1:103:A:GLN:HE21 | 4 | 0.31 | 0.1 | 0.26 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE1 | 4 | 0.31 | 0.27 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE2 | 4 | 0.31 | 0.27 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE3 | 4 | 0.31 | 0.27 | 0.15 |
| (1,443) | 1:135:A:LYS:H | 1:135:A:LYS:HE2 | 4 | 0.3 | 0.12 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,52) | 1:32:A:LEU:H | 1:32:A:LEU:HG | 4 | 0.29 | 0.1 | 0.31 |
| (1,305) | 1:31:A:VAL:H | 1:217:A:VAL:H | 4 | 0.29 | 0.17 | 0.22 |
| (1,1080) | 1:8:A:ILE:HG12 | 1:90:A:CYS:HA | 4 | 0.29 | 0.09 | 0.28 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG21 | 4 | 0.28 | 0.06 | 0.29 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG22 | 4 | 0.28 | 0.06 | 0.29 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG23 | 4 | 0.28 | 0.06 | 0.29 |
| (1,1730) | 1:108:A:PHE:HA | 1:109:A:GLU:HG2 | 4 | 0.28 | 0.12 | 0.28 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD21 | 4 | 0.27 | 0.13 | 0.24 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD22 | 4 | 0.27 | 0.13 | 0.24 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD23 | 4 | 0.27 | 0.13 | 0.24 |
| (1,1805) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HB | 4 | 0.27 | 0.16 | 0.2 |
| (1,1805) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HB | 4 | 0.27 | 0.16 | 0.2 |
| (1,1805) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HB | 4 | 0.27 | 0.16 | 0.2 |
| (1,1805) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HB | 4 | 0.27 | 0.16 | 0.2 |
| (1,1805) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HB | 4 | 0.27 | 0.16 | 0.2 |
| (1,1805) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HB | 4 | 0.27 | 0.16 | 0.2 |
| (1,234) | 1:10:A:PRO:HA | 1:28:A:PHE:H | 4 | 0.27 | 0.05 | 0.26 |
| (1,518) | 1:3:A:LEU:H | 1:87:A:GLY:H | 4 | 0.27 | 0.13 | 0.25 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD11 | 4 | 0.26 | 0.13 | 0.2 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD12 | 4 | 0.26 | 0.13 | 0.2 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD13 | 4 | 0.26 | 0.13 | 0.2 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD21 | 4 | 0.26 | 0.13 | 0.2 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD22 | 4 | 0.26 | 0.13 | 0.2 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD23 | 4 | 0.26 | 0.13 | 0.2 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD1 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD2 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD1 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD2 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD1 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD2 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD1 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD2 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD1 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD2 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD1 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD2 | 4 | 0.26 | 0.07 | 0.26 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD11 | 4 | 0.26 | 0.12 | 0.23 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD12 | 4 | 0.26 | 0.12 | 0.23 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD13 | 4 | 0.26 | 0.12 | 0.23 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG11 | 4 | 0.26 | 0.1 | 0.28 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG12 | 4 | 0.26 | 0.1 | 0.28 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG13 | 4 | 0.26 | 0.1 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG21 | 4 | 0.26 | 0.1 | 0.28 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG22 | 4 | 0.26 | 0.1 | 0.28 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG23 | 4 | 0.26 | 0.1 | 0.28 |
| (1,1007) | 1:17:A:LEU:HA | 1:17:A:LEU:HG | 4 | 0.24 | 0.03 | 0.23 |
| (1,1721) | 1:225:A:GLU:HG2 | 1:226:A:HIS:H | 4 | 0.24 | 0.08 | 0.26 |
| (1,1663) | 1:23:A:ALA:HA | 1:108:A:PHE:HB2 | 4 | 0.24 | 0.12 | 0.2 |
| (1,416) | 1:193:A:LEU:HD11 | 1:197:A:ALA:H | 4 | 0.24 | 0.12 | 0.18 |
| (1,416) | 1:193:A:LEU:HD12 | 1:197:A:ALA:H | 4 | 0.24 | 0.12 | 0.18 |
| (1,416) | 1:193:A:LEU:HD13 | 1:197:A:ALA:H | 4 | 0.24 | 0.12 | 0.18 |
| (1,416) | 1:193:A:LEU:HD21 | 1:197:A:ALA:H | 4 | 0.24 | 0.12 | 0.18 |
| (1,416) | 1:193:A:LEU:HD22 | 1:197:A:ALA:H | 4 | 0.24 | 0.12 | 0.18 |
| (1,416) | 1:193:A:LEU:HD23 | 1:197:A:ALA:H | 4 | 0.24 | 0.12 | 0.18 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB1 | 4 | 0.24 | 0.15 | 0.16 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB2 | 4 | 0.24 | 0.15 | 0.16 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB3 | 4 | 0.24 | 0.15 | 0.16 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD1 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD2 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD1 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD2 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD1 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD2 | 4 | 0.23 | 0.05 | 0.22 |
| (1,1157) | 1:28:A:PHE:HA | 1:217:A:VAL:HA | 4 | 0.22 | 0.06 | 0.2 |
| (1,122) | 1:99:A:VAL:HG11 | 1:102:A:ASN:H | 4 | 0.22 | 0.09 | 0.2 |
| (1,122) | 1:99:A:VAL:HG12 | 1:102:A:ASN:H | 4 | 0.22 | 0.09 | 0.2 |
| (1,122) | 1:99:A:VAL:HG13 | 1:102:A:ASN:H | 4 | 0.22 | 0.09 | 0.2 |
| (1,122) | 1:99:A:VAL:HG21 | 1:102:A:ASN:H | 4 | 0.22 | 0.09 | 0.2 |
| (1,122) | 1:99:A:VAL:HG22 | 1:102:A:ASN:H | 4 | 0.22 | 0.09 | 0.2 |
| (1,122) | 1:99:A:VAL:HG23 | 1:102:A:ASN:H | 4 | 0.22 | 0.09 | 0.2 |
| (1,1238) | 1:55:A:LEU:HG | 1:160:A:PHE:HA | 4 | 0.21 | 0.09 | 0.21 |
| (1,317) | 1:206:A:GLU:H | 1:208:A:GLU:H | 4 | 0.21 | 0.1 | 0.16 |
| (1,1707) | 1:35:A:GLU:HG2 | 1:36:A:GLU:H | 4 | 0.2 | 0.03 | 0.19 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG11 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG12 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG13 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG21 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG22 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG23 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG11 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG12 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG13 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG21 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG22 | 4 | 0.2 | 0.04 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG23 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG11 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG12 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG13 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG21 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG22 | 4 | 0.2 | 0.04 | 0.2 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG23 | 4 | 0.2 | 0.04 | 0.2 |
| (1,731) | 1:194:A:LEU:H | 1:196:A:ASP:H | 4 | 0.2 | 0.07 | 0.18 |
| (1,1965) | 1:49:A:LEU:HD11 | 1:219:A:LEU:H | 4 | 0.2 | 0.08 | 0.18 |
| (1,1965) | 1:49:A:LEU:HD12 | 1:219:A:LEU:H | 4 | 0.2 | 0.08 | 0.18 |
| (1,1965) | 1:49:A:LEU:HD13 | 1:219:A:LEU:H | 4 | 0.2 | 0.08 | 0.18 |
| (1,1965) | 1:49:A:LEU:HD21 | 1:219:A:LEU:H | 4 | 0.2 | 0.08 | 0.18 |
| (1,1965) | 1:49:A:LEU:HD22 | 1:219:A:LEU:H | 4 | 0.2 | 0.08 | 0.18 |
| (1,1965) | 1:49:A:LEU:HD23 | 1:219:A:LEU:H | 4 | 0.2 | 0.08 | 0.18 |
| (1,1572) | 1:221:A:LYS:HD2 | 1:222:A:ALA:H | 4 | 0.2 | 0.05 | 0.22 |
| (1,1693) | 1:127:A:GLU:HG2 | 1:130:A:ALA:H | 4 | 0.2 | 0.04 | 0.2 |
| (1,246) | 1:164:A:LEU:HD11 | 1:175:A:LEU:H | 4 | 0.19 | 0.02 | 0.19 |
| (1,246) | 1:164:A:LEU:HD12 | 1:175:A:LEU:H | 4 | 0.19 | 0.02 | 0.19 |
| (1,246) | 1:164:A:LEU:HD13 | 1:175:A:LEU:H | 4 | 0.19 | 0.02 | 0.19 |
| (1,246) | 1:164:A:LEU:HD21 | 1:175:A:LEU:H | 4 | 0.19 | 0.02 | 0.19 |
| (1,246) | 1:164:A:LEU:HD22 | 1:175:A:LEU:H | 4 | 0.19 | 0.02 | 0.19 |
| (1,246) | 1:164:A:LEU:HD23 | 1:175:A:LEU:H | 4 | 0.19 | 0.02 | 0.19 |
| (1,859) | 1:155:A:ASP:H | 1:155:A:ASP:HB2 | 4 | 0.18 | 0.02 | 0.18 |
| (1,1500) | 1:130:A:ALA:HB1 | 1:132:A:CYS:H | 4 | 0.17 | 0.05 | 0.16 |
| (1,1500) | 1:130:A:ALA:HB2 | 1:132:A:CYS:H | 4 | 0.17 | 0.05 | 0.16 |
| (1,1500) | 1:130:A:ALA:HB3 | 1:132:A:CYS:H | 4 | 0.17 | 0.05 | 0.16 |
| (1,2007) | 1:58:A:GLN:HB2 | 1:59:A:HIS:H | 4 | 0.17 | 0.03 | 0.18 |
| (1,911) | 1:137:A:GLU:HA | 1:140:A:GLN:H | 4 | 0.16 | 0.05 | 0.14 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG11 | 4 | 0.16 | 0.05 | 0.14 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG12 | 4 | 0.16 | 0.05 | 0.14 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG13 | 4 | 0.16 | 0.05 | 0.14 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG21 | 4 | 0.16 | 0.05 | 0.14 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG22 | 4 | 0.16 | 0.05 | 0.14 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG23 | 4 | 0.16 | 0.05 | 0.14 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB1 | 4 | 0.15 | 0.06 | 0.12 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB2 | 4 | 0.15 | 0.06 | 0.12 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB3 | 4 | 0.15 | 0.06 | 0.12 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD21 | 4 | 0.15 | 0.03 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD22 | 4 | 0.15 | 0.03 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD23 | 4 | 0.15 | 0.03 | 0.13 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE1 | 4 | 0.13 | 0.03 | 0.12 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE2 | 4 | 0.13 | 0.03 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,253) | 1:186:A:GLY:H | 1:187:A:ALA:H | 4 | 0.12 | 0.01 | 0.12 |
| (1,672) | 1:76:A:SER:H | 1:77:A:PRO:HD2 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1051) | 1:23:A:ALA:HB1 | 1:107:A:GLY:H | 3 | 0.7 | 0.16 | 0.73 |
| (1,1051) | 1:23:A:ALA:HB2 | 1:107:A:GLY:H | 3 | 0.7 | 0.16 | 0.73 |
| (1,1051) | 1:23:A:ALA:HB3 | 1:107:A:GLY:H | 3 | 0.7 | 0.16 | 0.73 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD1 | 3 | 0.56 | 0.3 | 0.74 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD2 | 3 | 0.56 | 0.3 | 0.74 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG21 | 3 | 0.54 | 0.34 | 0.55 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG22 | 3 | 0.54 | 0.34 | 0.55 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG23 | 3 | 0.54 | 0.34 | 0.55 |
| (1,1410) | 1:137:A:GLU:H | 1:140:A:GLN:HB2 | 3 | 0.5 | 0.16 | 0.53 |
| (1,801) | 1:56:A:THR:HG21 | 1:57:A:ALA:HA | 3 | 0.47 | 0.17 | 0.43 |
| (1,801) | 1:56:A:THR:HG22 | 1:57:A:ALA:HA | 3 | 0.47 | 0.17 | 0.43 |
| (1,801) | 1:56:A:THR:HG23 | 1:57:A:ALA:HA | 3 | 0.47 | 0.17 | 0.43 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG11 | 3 | 0.46 | 0.03 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG12 | 3 | 0.46 | 0.03 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG13 | 3 | 0.46 | 0.03 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG21 | 3 | 0.46 | 0.03 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG22 | 3 | 0.46 | 0.03 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG23 | 3 | 0.46 | 0.03 | 0.44 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD1 | 3 | 0.44 | 0.21 | 0.35 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD2 | 3 | 0.44 | 0.21 | 0.35 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD11 | 3 | 0.42 | 0.24 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD12 | 3 | 0.42 | 0.24 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD13 | 3 | 0.42 | 0.24 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD21 | 3 | 0.42 | 0.24 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD22 | 3 | 0.42 | 0.24 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD23 | 3 | 0.42 | 0.24 | 0.43 |
| (1,1121) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HG2 | 3 | 0.41 | 0.15 | 0.47 |
| (1,1121) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HG2 | 3 | 0.41 | 0.15 | 0.47 |
| (1,1121) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HG2 | 3 | 0.41 | 0.15 | 0.47 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE21 | 3 | 0.4 | 0.32 | 0.23 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE22 | 3 | 0.4 | 0.32 | 0.23 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD21 | 3 | 0.39 | 0.15 | 0.38 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD22 | 3 | 0.39 | 0.15 | 0.38 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD23 | 3 | 0.39 | 0.15 | 0.38 |
| (1,1211) | 1:52:A:LEU:HA | 1:215:A:SER:HB2 | 3 | 0.37 | 0.33 | 0.15 |
| (1,2192) | 1:129:A:ARG:HG2 | 1:132:A:CYS:HB2 | 3 | 0.37 | 0.17 | 0.31 |
| (1,574) | 1:164:A:LEU:HG | 1:175:A:LEU:H | 3 | 0.35 | 0.09 | 0.31 |
| (1,1673) | 1:115:A:LYS:HE2 | 1:116:A:GLN:HA | 3 | 0.35 | 0.15 | 0.36 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD11 | 3 | 0.34 | 0.19 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD12 | 3 | 0.34 | 0.19 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD13 | 3 | 0.34 | 0.19 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD21 | 3 | 0.34 | 0.19 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD22 | 3 | 0.34 | 0.19 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD23 | 3 | 0.34 | 0.19 | 0.3 |
| (1,2210) | 1:136:A:ASN:HD21 | 1:137:A:GLU:HB2 | 3 | 0.34 | 0.33 | 0.12 |
| (1,2210) | 1:136:A:ASN:HD22 | 1:137:A:GLU:HB2 | 3 | 0.34 | 0.33 | 0.12 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD11 | 3 | 0.34 | 0.06 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD12 | 3 | 0.34 | 0.06 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD13 | 3 | 0.34 | 0.06 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD21 | 3 | 0.34 | 0.06 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD22 | 3 | 0.34 | 0.06 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD23 | 3 | 0.34 | 0.06 | 0.36 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE1 | 3 | 0.33 | 0.15 | 0.41 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE2 | 3 | 0.33 | 0.15 | 0.41 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE1 | 3 | 0.33 | 0.15 | 0.41 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE2 | 3 | 0.33 | 0.15 | 0.41 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE1 | 3 | 0.33 | 0.15 | 0.41 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE2 | 3 | 0.33 | 0.15 | 0.41 |
| (1,557) | 1:74:A:GLU:HB2 | 1:75:A:VAL:H | 3 | 0.32 | 0.02 | 0.32 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE1 | 3 | 0.31 | 0.16 | 0.21 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE2 | 3 | 0.31 | 0.16 | 0.21 |
| (1,254) | 1:209:A:GLN:HG2 | 1:210:A:GLY:H | 3 | 0.3 | 0.15 | 0.26 |
| (1,1483) | 1:34:A:LEU:HD11 | 1:201:A:CYS:HB2 | 3 | 0.3 | 0.22 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD12 | 1:201:A:CYS:HB2 | 3 | 0.3 | 0.22 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD13 | 1:201:A:CYS:HB2 | 3 | 0.3 | 0.22 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD21 | 1:201:A:CYS:HB2 | 3 | 0.3 | 0.22 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD22 | 1:201:A:CYS:HB2 | 3 | 0.3 | 0.22 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD23 | 1:201:A:CYS:HB2 | 3 | 0.3 | 0.22 | 0.16 |
| (1,491) | 1:211:A:GLU:HA | 1:212:A:VAL:H | 3 | 0.3 | 0.07 | 0.25 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE21 | 3 | 0.29 | 0.17 | 0.21 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE22 | 3 | 0.29 | 0.17 | 0.21 |
| (1,163) | 1:151:A:GLN:HB2 | 1:152:A:CYS:H | 3 | 0.29 | 0.08 | 0.25 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB1 | 3 | 0.29 | 0.2 | 0.19 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB2 | 3 | 0.29 | 0.2 | 0.19 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB3 | 3 | 0.29 | 0.2 | 0.19 |
| (1,361) | 1:15:A:LYS:H | 1:15:A:LYS:HE2 | 3 | 0.28 | 0.09 | 0.3 |
| (1,1295) | 1:3:A:LEU:HG | 1:4:A:LYS:H | 3 | 0.27 | 0.16 | 0.22 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG21 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG22 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG23 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG21 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG22 | 3 | 0.27 | 0.07 | 0.31 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG23 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG21 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG22 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG23 | 3 | 0.27 | 0.07 | 0.31 |
| (1,1650) | 1:153:A:ARG:H | 1:153:A:ARG:HG2 | 3 | 0.27 | 0.04 | 0.24 |
| (1,1045) | 1:67:A:ILE:HA | 1:70:A:LEU:HB2 | 3 | 0.26 | 0.12 | 0.29 |
| (1,368) | 1:18:A:TYR:H | 1:19:A:ARG:HB2 | 3 | 0.26 | 0.03 | 0.26 |
| (1,1588) | 1:100:A:ALA:HB1 | 1:118:A:LEU:HG | 3 | 0.25 | 0.09 | 0.26 |
| (1,1588) | 1:100:A:ALA:HB2 | 1:118:A:LEU:HG | 3 | 0.25 | 0.09 | 0.26 |
| (1,1588) | 1:100:A:ALA:HB3 | 1:118:A:LEU:HG | 3 | 0.25 | 0.09 | 0.26 |
| (1,745) | 1:55:A:LEU:H | 1:160:A:PHE:HB2 | 3 | 0.24 | 0.11 | 0.22 |
| (1,1466) | 1:19:A:ARG:HD2 | 1:145:A:ALA:H | 3 | 0.24 | 0.11 | 0.22 |
| (1,1745) | 1:31:A:VAL:HB | 1:218:A:ALA:H | 3 | 0.24 | 0.11 | 0.23 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE1 | 3 | 0.24 | 0.02 | 0.25 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE2 | 3 | 0.24 | 0.02 | 0.25 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD1 | 3 | 0.23 | 0.13 | 0.17 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD2 | 3 | 0.23 | 0.13 | 0.17 |
| (1,1962) | 1:49:A:LEU:HD11 | 1:198:A:ALA:HA | 3 | 0.23 | 0.04 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD12 | 1:198:A:ALA:HA | 3 | 0.23 | 0.04 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD13 | 1:198:A:ALA:HA | 3 | 0.23 | 0.04 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD21 | 1:198:A:ALA:HA | 3 | 0.23 | 0.04 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD22 | 1:198:A:ALA:HA | 3 | 0.23 | 0.04 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD23 | 1:198:A:ALA:HA | 3 | 0.23 | 0.04 | 0.24 |
| (1,940) | 1:154:A:VAL:HG11 | 1:155:A:ASP:HA | 3 | 0.22 | 0.15 | 0.12 |
| (1,940) | 1:154:A:VAL:HG12 | 1:155:A:ASP:HA | 3 | 0.22 | 0.15 | 0.12 |
| (1,940) | 1:154:A:VAL:HG13 | 1:155:A:ASP:HA | 3 | 0.22 | 0.15 | 0.12 |
| (1,940) | 1:154:A:VAL:HG21 | 1:155:A:ASP:HA | 3 | 0.22 | 0.15 | 0.12 |
| (1,940) | 1:154:A:VAL:HG22 | 1:155:A:ASP:HA | 3 | 0.22 | 0.15 | 0.12 |
| (1,940) | 1:154:A:VAL:HG23 | 1:155:A:ASP:HA | 3 | 0.22 | 0.15 | 0.12 |
| (1,1718) | 1:210:A:GLY:H | 1:211:A:GLU:HG2 | 3 | 0.22 | 0.06 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HB | 3 | 0.22 | 0.09 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HB | 3 | 0.22 | 0.09 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HB | 3 | 0.22 | 0.09 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG21 | 1:168:A:VAL:HB | 3 | 0.22 | 0.09 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG22 | 1:168:A:VAL:HB | 3 | 0.22 | 0.09 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG23 | 1:168:A:VAL:HB | 3 | 0.22 | 0.09 | 0.21 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE1 | 3 | 0.22 | 0.08 | 0.23 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE2 | 3 | 0.22 | 0.08 | 0.23 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE3 | 3 | 0.22 | 0.08 | 0.23 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD11 | 3 | 0.21 | 0.07 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD12 | 3 | 0.21 | 0.07 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD13 | 3 | 0.21 | 0.07 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD21 | 3 | 0.21 | 0.07 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD22 | 3 | 0.21 | 0.07 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD23 | 3 | 0.21 | 0.07 | 0.25 |
| (1,427) | 1:212:A:VAL:HG11 | 1:214:A:PHE:H | 3 | 0.21 | 0.12 | 0.13 |
| (1,427) | 1:212:A:VAL:HG12 | 1:214:A:PHE:H | 3 | 0.21 | 0.12 | 0.13 |
| (1,427) | 1:212:A:VAL:HG13 | 1:214:A:PHE:H | 3 | 0.21 | 0.12 | 0.13 |
| (1,427) | 1:212:A:VAL:HG21 | 1:214:A:PHE:H | 3 | 0.21 | 0.12 | 0.13 |
| (1,427) | 1:212:A:VAL:HG22 | 1:214:A:PHE:H | 3 | 0.21 | 0.12 | 0.13 |
| (1,427) | 1:212:A:VAL:HG23 | 1:214:A:PHE:H | 3 | 0.21 | 0.12 | 0.13 |
| (1,1724) | 1:74:A:GLU:HG2 | 1:75:A:VAL:H | 3 | 0.21 | 0.07 | 0.2 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD11 | 3 | 0.2 | 0.03 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD12 | 3 | 0.2 | 0.03 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD13 | 3 | 0.2 | 0.03 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD21 | 3 | 0.2 | 0.03 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD22 | 3 | 0.2 | 0.03 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD23 | 3 | 0.2 | 0.03 | 0.18 |
| (1,727) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE22 | 3 | 0.2 | 0.05 | 0.18 |
| (1,727) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE22 | 3 | 0.2 | 0.05 | 0.18 |
| (1,727) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE22 | 3 | 0.2 | 0.05 | 0.18 |
| (1,1488) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HA | 3 | 0.2 | 0.13 | 0.11 |
| (1,377) | 1:31:A:VAL:HG11 | 1:32:A:LEU:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,377) | 1:31:A:VAL:HG12 | 1:32:A:LEU:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,377) | 1:31:A:VAL:HG13 | 1:32:A:LEU:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,377) | 1:31:A:VAL:HG21 | 1:32:A:LEU:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,377) | 1:31:A:VAL:HG22 | 1:32:A:LEU:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,377) | 1:31:A:VAL:HG23 | 1:32:A:LEU:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,2277) | 1:167:A:ASN:HD21 | 1:172:A:LEU:HB2 | 3 | 0.2 | 0.03 | 0.18 |
| (1,2277) | 1:167:A:ASN:HD22 | 1:172:A:LEU:HB2 | 3 | 0.2 | 0.03 | 0.18 |
| (1,2193) | 1:131:A:LYS:H | 1:132:A:CYS:HB2 | 3 | 0.19 | 0.09 | 0.15 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD11 | 3 | 0.19 | 0.08 | 0.14 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD12 | 3 | 0.19 | 0.08 | 0.14 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD13 | 3 | 0.19 | 0.08 | 0.14 |
| (1,1465) | 1:212:A:VAL:HB | 1:213:A:ARG:HD2 | 3 | 0.18 | 0.08 | 0.14 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG11 | 3 | 0.17 | 0.04 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG12 | 3 | 0.17 | 0.04 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG13 | 3 | 0.17 | 0.04 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG21 | 3 | 0.17 | 0.04 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG22 | 3 | 0.17 | 0.04 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG23 | 3 | 0.17 | 0.04 | 0.16 |
| (1,543) | 1:60:A:GLU:H | 1:62:A:PHE:H | 3 | 0.17 | 0.03 | 0.18 |
| (1,684) | 1:168:A:VAL:HA | 1:171:A:HIS:H | 3 | 0.17 | 0.04 | 0.19 |
| (1,535) | 1:117:A:PHE:HA | 1:120:A:GLU:H | 3 | 0.16 | 0.04 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1356) | 1:117:A:PHE:HA | 1:119:A:SER:H | 3 | 0.16 | 0.04 | 0.18 |
| (1,1658) | 1:158:A:VAL:HB | 1:159:A:ASN:H | 3 | 0.16 | 0.06 | 0.13 |
| (1,2362) | 1:219:A:LEU:HD11 | 1:222:A:ALA:H | 3 | 0.16 | 0.03 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD12 | 1:222:A:ALA:H | 3 | 0.16 | 0.03 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD13 | 1:222:A:ALA:H | 3 | 0.16 | 0.03 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD21 | 1:222:A:ALA:H | 3 | 0.16 | 0.03 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD22 | 1:222:A:ALA:H | 3 | 0.16 | 0.03 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD23 | 1:222:A:ALA:H | 3 | 0.16 | 0.03 | 0.17 |
| (1,1112) | 1:151:A:GLN:HA | 1:151:A:GLN:HG2 | 3 | 0.15 | 0.0 | 0.15 |
| (1,1350) | 1:156:A:ASP:HB2 | 1:158:A:VAL:HA | 3 | 0.15 | 0.07 | 0.1 |
| (1,909) | 1:209:A:GLN:H | 1:209:A:GLN:HG2 | 3 | 0.15 | 0.02 | 0.16 |
| (1,1400) | 1:6:A:MET:HA | 1:7:A:GLU:HA | 3 | 0.15 | 0.03 | 0.17 |
| (1,630) | 1:112:A:SER:HA | 1:114:A:LEU:H | 3 | 0.15 | 0.01 | 0.15 |
| (1,18) | 1:18:A:TYR:HD1 | 1:19:A:ARG:H | 3 | 0.14 | 0.02 | 0.14 |
| (1,18) | 1:18:A:TYR:HD2 | 1:19:A:ARG:H | 3 | 0.14 | 0.02 | 0.14 |
| (1,382) | 1:120:A:GLU:H | 1:122:A:GLU:H | 3 | 0.14 | 0.02 | 0.15 |
| (1,2018) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HD2 | 3 | 0.14 | 0.02 | 0.13 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB1 | 3 | 0.14 | 0.02 | 0.13 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB2 | 3 | 0.14 | 0.02 | 0.13 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB3 | 3 | 0.14 | 0.02 | 0.13 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD11 | 3 | 0.14 | 0.04 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD12 | 3 | 0.14 | 0.04 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD13 | 3 | 0.14 | 0.04 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD21 | 3 | 0.14 | 0.04 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD22 | 3 | 0.14 | 0.04 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD23 | 3 | 0.14 | 0.04 | 0.12 |
| (1,1808) | 1:3:A:LEU:HD11 | 1:140:A:GLN:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD12 | 1:140:A:GLN:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD13 | 1:140:A:GLN:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD21 | 1:140:A:GLN:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD22 | 1:140:A:GLN:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD23 | 1:140:A:GLN:H | 3 | 0.13 | 0.02 | 0.13 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG11 | 3 | 0.13 | 0.02 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG12 | 3 | 0.13 | 0.02 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG13 | 3 | 0.13 | 0.02 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG21 | 3 | 0.13 | 0.02 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG22 | 3 | 0.13 | 0.02 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG23 | 3 | 0.13 | 0.02 | 0.14 |
| (1,2079) | 1:82:A:MET:HE1 | 1:93:A:ILE:HG12 | 3 | 0.12 | 0.01 | 0.12 |
| (1,2079) | 1:82:A:MET:HE2 | 1:93:A:ILE:HG12 | 3 | 0.12 | 0.01 | 0.12 |
| (1,2079) | 1:82:A:MET:HE3 | 1:93:A:ILE:HG12 | 3 | 0.12 | 0.01 | 0.12 |
| (1,333) | 1:98:A:ALA:H | 1:100:A:ALA:H | 3 | 0.12 | 0.01 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,634) | 1:32:A:LEU:H | 1:34:A:LEU:H | 3 | 0.11 | 0.01 | 0.12 |
| (1,968) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 2 | 0.68 | 0.09 | 0.68 |
| (1,968) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 2 | 0.68 | 0.09 | 0.68 |
| (1,968) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 2 | 0.68 | 0.09 | 0.68 |
| (1,974) | 1:82:A:MET:HE1 | 1:92:A:THR:HB | 2 | 0.68 | 0.29 | 0.68 |
| (1,974) | 1:82:A:MET:HE2 | 1:92:A:THR:HB | 2 | 0.68 | 0.29 | 0.68 |
| (1,974) | 1:82:A:MET:HE3 | 1:92:A:THR:HB | 2 | 0.68 | 0.29 | 0.68 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD21 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD22 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD23 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD21 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD22 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD23 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD21 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD22 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD23 | 2 | 0.57 | 0.18 | 0.57 |
| (1,1830) | 1:7:A:GLU:HG2 | 1:8:A:ILE:HB | 2 | 0.55 | 0.03 | 0.55 |
| (1,1237) | 1:55:A:LEU:HG | 1:56:A:THR:HA | 2 | 0.48 | 0.12 | 0.48 |
| (1,1876) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE21 | 2 | 0.48 | 0.07 | 0.48 |
| (1,1876) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 2 | 0.48 | 0.07 | 0.48 |
| (1,1876) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE21 | 2 | 0.48 | 0.07 | 0.48 |
| (1,1876) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 2 | 0.48 | 0.07 | 0.48 |
| (1,1876) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE21 | 2 | 0.48 | 0.07 | 0.48 |
| (1,1876) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 2 | 0.48 | 0.07 | 0.48 |
| (1,80) | 1:52:A:LEU:H | 1:53:A:PHE:HD1 | 2 | 0.46 | 0.16 | 0.46 |
| (1,80) | 1:52:A:LEU:H | 1:53:A:PHE:HD2 | 2 | 0.46 | 0.16 | 0.46 |
| (1,820) | 1:96:A:ILE:HA | 1:99:A:VAL:HB | 2 | 0.46 | 0.12 | 0.46 |
| (1,2098) | 1:99:A:VAL:HA | 1:102:A:ASN:HD21 | 2 | 0.46 | 0.31 | 0.46 |
| (1,2098) | 1:99:A:VAL:HA | 1:102:A:ASN:HD22 | 2 | 0.46 | 0.31 | 0.46 |
| (1,964) | 1:124:A:MET:HE1 | 1:132:A:CYS:H | 2 | 0.46 | 0.05 | 0.46 |
| (1,964) | 1:124:A:MET:HE2 | 1:132:A:CYS:H | 2 | 0.46 | 0.05 | 0.46 |
| (1,964) | 1:124:A:MET:HE3 | 1:132:A:CYS:H | 2 | 0.46 | 0.05 | 0.46 |
| (1,1382) | 1:70:A:LEU:HG | 1:72:A:GLY:HA2 | 2 | 0.45 | 0.04 | 0.45 |
| (1,582) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD21 | 2 | 0.43 | 0.14 | 0.43 |
| (1,582) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD21 | 2 | 0.43 | 0.14 | 0.43 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD11 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD12 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD13 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD11 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD12 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD13 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD11 | 2 | 0.42 | 0.15 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD12 | 2 | 0.42 | 0.15 | 0.42 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD13 | 2 | 0.42 | 0.15 | 0.42 |
| (1,1188) | 1:36:A:GLU:H | 1:38:A:SER:HB2 | 2 | 0.4 | 0.27 | 0.4 |
| (1,1519) | 1:16:A:VAL:HB | 1:95:A:LEU:HB2 | 2 | 0.4 | 0.24 | 0.4 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD11 | 2 | 0.4 | 0.12 | 0.4 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD12 | 2 | 0.4 | 0.12 | 0.4 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD13 | 2 | 0.4 | 0.12 | 0.4 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD21 | 2 | 0.4 | 0.12 | 0.4 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD22 | 2 | 0.4 | 0.12 | 0.4 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD23 | 2 | 0.4 | 0.12 | 0.4 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG21 | 2 | 0.39 | 0.11 | 0.39 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG22 | 2 | 0.39 | 0.11 | 0.39 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG23 | 2 | 0.39 | 0.11 | 0.39 |
| (1,351) | 1:208:A:GLU:HA | 1:209:A:GLN:H | 2 | 0.39 | 0.03 | 0.39 |
| (1,586) | 1:67:A:ILE:HD11 | 1:176:A:ASP:H | 2 | 0.38 | 0.16 | 0.38 |
| (1,586) | 1:67:A:ILE:HD12 | 1:176:A:ASP:H | 2 | 0.38 | 0.16 | 0.38 |
| (1,586) | 1:67:A:ILE:HD13 | 1:176:A:ASP:H | 2 | 0.38 | 0.16 | 0.38 |
| (1,56) | 1:31:A:VAL:HG11 | 1:33:A:GLY:H | 2 | 0.37 | 0.02 | 0.37 |
| (1,56) | 1:31:A:VAL:HG12 | 1:33:A:GLY:H | 2 | 0.37 | 0.02 | 0.37 |
| (1,56) | 1:31:A:VAL:HG13 | 1:33:A:GLY:H | 2 | 0.37 | 0.02 | 0.37 |
| (1,56) | 1:31:A:VAL:HG21 | 1:33:A:GLY:H | 2 | 0.37 | 0.02 | 0.37 |
| (1,56) | 1:31:A:VAL:HG22 | 1:33:A:GLY:H | 2 | 0.37 | 0.02 | 0.37 |
| (1,56) | 1:31:A:VAL:HG23 | 1:33:A:GLY:H | 2 | 0.37 | 0.02 | 0.37 |
| (1,502) | 1:224:A:LEU:HG | 1:225:A:GLU:H | 2 | 0.37 | 0.06 | 0.37 |
| (1,933) | 1:11:A:GLU:HA | 1:11:A:GLU:HG2 | 2 | 0.37 | 0.01 | 0.37 |
| (1,224) | 1:167:A:ASN:HD21 | 1:190:A:GLU:HA | 2 | 0.36 | 0.11 | 0.36 |
| (1,350) | 1:208:A:GLU:HG2 | 1:209:A:GLN:H | 2 | 0.36 | 0.15 | 0.36 |
| (1,1622) | 1:51:A:LEU:HD11 | 1:53:A:PHE:HB2 | 2 | 0.36 | 0.08 | 0.36 |
| (1,1622) | 1:51:A:LEU:HD12 | 1:53:A:PHE:HB2 | 2 | 0.36 | 0.08 | 0.36 |
| (1,1622) | 1:51:A:LEU:HD13 | 1:53:A:PHE:HB2 | 2 | 0.36 | 0.08 | 0.36 |
| (1,285) | 1:9:A:ASN:HB2 | 1:12:A:MET:H | 2 | 0.34 | 0.0 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD11 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD12 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD13 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD21 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD22 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD23 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD11 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD12 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD13 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD21 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD22 | 2 | 0.34 | 0.19 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD23 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD11 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD12 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD13 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD21 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD22 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD23 | 2 | 0.34 | 0.19 | 0.34 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD11 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD12 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD13 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD21 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD22 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD23 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1874) | 1:17:A:LEU:HD11 | 1:95:A:LEU:HB2 | 2 | 0.34 | 0.13 | 0.34 |
| (1,1874) | 1:17:A:LEU:HD12 | 1:95:A:LEU:HB2 | 2 | 0.34 | 0.13 | 0.34 |
| (1,1874) | 1:17:A:LEU:HD13 | 1:95:A:LEU:HB2 | 2 | 0.34 | 0.13 | 0.34 |
| (1,1874) | 1:17:A:LEU:HD21 | 1:95:A:LEU:HB2 | 2 | 0.34 | 0.13 | 0.34 |
| (1,1874) | 1:17:A:LEU:HD22 | 1:95:A:LEU:HB2 | 2 | 0.34 | 0.13 | 0.34 |
| (1,1874) | 1:17:A:LEU:HD23 | 1:95:A:LEU:HB2 | 2 | 0.34 | 0.13 | 0.34 |
| (1,2290) | 1:168:A:VAL:HG11 | 1:169:A:ASP:HA | 2 | 0.33 | 0.02 | 0.33 |
| (1,2290) | 1:168:A:VAL:HG12 | 1:169:A:ASP:HA | 2 | 0.33 | 0.02 | 0.33 |
| (1,2290) | 1:168:A:VAL:HG13 | 1:169:A:ASP:HA | 2 | 0.33 | 0.02 | 0.33 |
| (1,2290) | 1:168:A:VAL:HG21 | 1:169:A:ASP:HA | 2 | 0.33 | 0.02 | 0.33 |
| (1,2290) | 1:168:A:VAL:HG22 | 1:169:A:ASP:HA | 2 | 0.33 | 0.02 | 0.33 |
| (1,2290) | 1:168:A:VAL:HG23 | 1:169:A:ASP:HA | 2 | 0.33 | 0.02 | 0.33 |
| (1,30) | 1:23:A:ALA:H | 1:109:A:GLU:H | 2 | 0.32 | 0.09 | 0.32 |
| (1,576) | 1:171:A:HIS:HD2 | 1:172:A:LEU:H | 2 | 0.32 | 0.02 | 0.32 |
| (1,458) | 1:156:A:ASP:HA | 1:158:A:VAL:H | 2 | 0.32 | 0.14 | 0.32 |
| (1,2062) | 1:79:A:VAL:HG11 | 1:168:A:VAL:H | 2 | 0.32 | 0.07 | 0.32 |
| (1,2062) | 1:79:A:VAL:HG12 | 1:168:A:VAL:H | 2 | 0.32 | 0.07 | 0.32 |
| (1,2062) | 1:79:A:VAL:HG13 | 1:168:A:VAL:H | 2 | 0.32 | 0.07 | 0.32 |
| (1,2062) | 1:79:A:VAL:HG21 | 1:168:A:VAL:H | 2 | 0.32 | 0.07 | 0.32 |
| (1,2062) | 1:79:A:VAL:HG22 | 1:168:A:VAL:H | 2 | 0.32 | 0.07 | 0.32 |
| (1,2062) | 1:79:A:VAL:HG23 | 1:168:A:VAL:H | 2 | 0.32 | 0.07 | 0.32 |
| (1,2032) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HD21 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HD22 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HD21 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HD22 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HD21 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HD22 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HD21 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HD22 | 2 | 0.31 | 0.03 | 0.31 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2032) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HD21 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HD22 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HD21 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2032) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HD22 | 2 | 0.31 | 0.03 | 0.31 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB1 | 2 | 0.31 | 0.19 | 0.31 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB2 | 2 | 0.31 | 0.19 | 0.31 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB3 | 2 | 0.31 | 0.19 | 0.31 |
| (1,193) | 1:192:A:THR:HA | 1:196:A:ASP:H | 2 | 0.31 | 0.04 | 0.31 |
| (1,1152) | 1:165:A:PHE:HD1 | 1:174:A:GLU:HA | 2 | 0.3 | 0.02 | 0.3 |
| (1,1152) | 1:165:A:PHE:HD2 | 1:174:A:GLU:HA | 2 | 0.3 | 0.02 | 0.3 |
| (1,1831) | 1:7:A:GLU:HG2 | 1:8:A:ILE:HG12 | 2 | 0.3 | 0.02 | 0.3 |
| (1,2226) | 1:148:A:GLN:H | 1:148:A:GLN:HG2 | 2 | 0.29 | 0.17 | 0.29 |
| (1,2320) | 1:183:A:VAL:HG11 | 1:185:A:HIS:HA | 2 | 0.29 | 0.09 | 0.29 |
| (1,2320) | 1:183:A:VAL:HG12 | 1:185:A:HIS:HA | 2 | 0.29 | 0.09 | 0.29 |
| (1,2320) | 1:183:A:VAL:HG13 | 1:185:A:HIS:HA | 2 | 0.29 | 0.09 | 0.29 |
| (1,2320) | 1:183:A:VAL:HG21 | 1:185:A:HIS:HA | 2 | 0.29 | 0.09 | 0.29 |
| (1,2320) | 1:183:A:VAL:HG22 | 1:185:A:HIS:HA | 2 | 0.29 | 0.09 | 0.29 |
| (1,2320) | 1:183:A:VAL:HG23 | 1:185:A:HIS:HA | 2 | 0.29 | 0.09 | 0.29 |
| (1,1587) | 1:121:A:THR:HG21 | 1:129:A:ARG:HD2 | 2 | 0.29 | 0.13 | 0.29 |
| (1,1587) | 1:121:A:THR:HG22 | 1:129:A:ARG:HD2 | 2 | 0.29 | 0.13 | 0.29 |
| (1,1587) | 1:121:A:THR:HG23 | 1:129:A:ARG:HD2 | 2 | 0.29 | 0.13 | 0.29 |
| (1,2345) | 1:200:A:VAL:HG11 | 1:203:A:GLU:HG2 | 2 | 0.29 | 0.08 | 0.29 |
| (1,2345) | 1:200:A:VAL:HG12 | 1:203:A:GLU:HG2 | 2 | 0.29 | 0.08 | 0.29 |
| (1,2345) | 1:200:A:VAL:HG13 | 1:203:A:GLU:HG2 | 2 | 0.29 | 0.08 | 0.29 |
| (1,2345) | 1:200:A:VAL:HG21 | 1:203:A:GLU:HG2 | 2 | 0.29 | 0.08 | 0.29 |
| (1,2345) | 1:200:A:VAL:HG22 | 1:203:A:GLU:HG2 | 2 | 0.29 | 0.08 | 0.29 |
| (1,2345) | 1:200:A:VAL:HG23 | 1:203:A:GLU:HG2 | 2 | 0.29 | 0.08 | 0.29 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD11 | 2 | 0.28 | 0.12 | 0.28 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD12 | 2 | 0.28 | 0.12 | 0.28 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD13 | 2 | 0.28 | 0.12 | 0.28 |
| (1,1203) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HD1 | 2 | 0.28 | 0.07 | 0.28 |
| (1,1203) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HD2 | 2 | 0.28 | 0.07 | 0.28 |
| (1,1203) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HD1 | 2 | 0.28 | 0.07 | 0.28 |
| (1,1203) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HD2 | 2 | 0.28 | 0.07 | 0.28 |
| (1,1203) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HD1 | 2 | 0.28 | 0.07 | 0.28 |
| (1,1203) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HD2 | 2 | 0.28 | 0.07 | 0.28 |
| (1,2202) | 1:136:A:ASN:H | 1:140:A:GLN:HE21 | 2 | 0.28 | 0.12 | 0.28 |
| (1,2202) | 1:136:A:ASN:H | 1:140:A:GLN:HE22 | 2 | 0.28 | 0.12 | 0.28 |
| (1,676) | 1:171:A:HIS:H | 1:171:A:HIS:HD2 | 2 | 0.27 | 0.14 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB1 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB2 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB3 | 2 | 0.27 | 0.1 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB1 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB2 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB3 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB1 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB2 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB3 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB1 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB2 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB3 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB1 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB2 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB3 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB1 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB2 | 2 | 0.27 | 0.1 | 0.27 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB3 | 2 | 0.27 | 0.1 | 0.27 |
| (1,1433) | 1:154:A:VAL:HG11 | 1:156:A:ASP:HA | 2 | 0.26 | 0.1 | 0.26 |
| (1,1433) | 1:154:A:VAL:HG12 | 1:156:A:ASP:HA | 2 | 0.26 | 0.1 | 0.26 |
| (1,1433) | 1:154:A:VAL:HG13 | 1:156:A:ASP:HA | 2 | 0.26 | 0.1 | 0.26 |
| (1,1433) | 1:154:A:VAL:HG21 | 1:156:A:ASP:HA | 2 | 0.26 | 0.1 | 0.26 |
| (1,1433) | 1:154:A:VAL:HG22 | 1:156:A:ASP:HA | 2 | 0.26 | 0.1 | 0.26 |
| (1,1433) | 1:154:A:VAL:HG23 | 1:156:A:ASP:HA | 2 | 0.26 | 0.1 | 0.26 |
| (1,1476) | 1:153:A:ARG:H | 1:153:A:ARG:HD2 | 2 | 0.26 | 0.04 | 0.26 |
| (1,465) | 1:168:A:VAL:H | 1:173:A:TYR:HE1 | 2 | 0.25 | 0.1 | 0.25 |
| (1,465) | 1:168:A:VAL:H | 1:173:A:TYR:HE2 | 2 | 0.25 | 0.1 | 0.25 |
| (1,1187) | 1:32:A:LEU:H | 1:38:A:SER:HB2 | 2 | 0.25 | 0.12 | 0.25 |
| (1,297) | 1:159:A:ASN:HA | 1:160:A:PHE:H | 2 | 0.24 | 0.08 | 0.24 |
| (1,765) | 1:192:A:THR:HA | 1:194:A:LEU:H | 2 | 0.24 | 0.06 | 0.24 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD11 | 2 | 0.24 | 0.03 | 0.24 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD12 | 2 | 0.24 | 0.03 | 0.24 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD13 | 2 | 0.24 | 0.03 | 0.24 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD21 | 2 | 0.24 | 0.03 | 0.24 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD22 | 2 | 0.24 | 0.03 | 0.24 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD23 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1056) | 1:52:A:LEU:HB2 | 1:214:A:PHE:HD1 | 2 | 0.24 | 0.1 | 0.24 |
| (1,1056) | 1:52:A:LEU:HB2 | 1:214:A:PHE:HD2 | 2 | 0.24 | 0.1 | 0.24 |
| (1,759) | 1:148:A:GLN:H | 1:148:A:GLN:HG2 | 2 | 0.24 | 0.02 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG21 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG22 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG23 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG21 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG22 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG23 | 2 | 0.24 | 0.06 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG21 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG22 | 2 | 0.24 | 0.06 | 0.24 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG23 | 2 | 0.24 | 0.06 | 0.24 |
| (1,229) | 1:213:A:ARG:H | 1:214:A:PHE:HA | 2 | 0.24 | 0.11 | 0.24 |
| (1,1672) | 1:115:A:LYS:HB2 | 1:115:A:LYS:HE2 | 2 | 0.24 | 0.0 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG21 | 2 | 0.24 | 0.0 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG22 | 2 | 0.24 | 0.0 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG23 | 2 | 0.24 | 0.0 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG21 | 2 | 0.24 | 0.0 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG22 | 2 | 0.24 | 0.0 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG23 | 2 | 0.24 | 0.0 | 0.24 |
| (1,910) | 1:39:A:LEU:HD11 | 1:195:A:LYS:HA | 2 | 0.23 | 0.0 | 0.23 |
| (1,910) | 1:39:A:LEU:HD12 | 1:195:A:LYS:HA | 2 | 0.23 | 0.0 | 0.23 |
| (1,910) | 1:39:A:LEU:HD13 | 1:195:A:LYS:HA | 2 | 0.23 | 0.0 | 0.23 |
| (1,2066) | 1:79:A:VAL:HG11 | 1:173:A:TYR:H | 2 | 0.23 | 0.11 | 0.23 |
| (1,2066) | 1:79:A:VAL:HG12 | 1:173:A:TYR:H | 2 | 0.23 | 0.11 | 0.23 |
| (1,2066) | 1:79:A:VAL:HG13 | 1:173:A:TYR:H | 2 | 0.23 | 0.11 | 0.23 |
| (1,2066) | 1:79:A:VAL:HG21 | 1:173:A:TYR:H | 2 | 0.23 | 0.11 | 0.23 |
| (1,2066) | 1:79:A:VAL:HG22 | 1:173:A:TYR:H | 2 | 0.23 | 0.11 | 0.23 |
| (1,2066) | 1:79:A:VAL:HG23 | 1:173:A:TYR:H | 2 | 0.23 | 0.11 | 0.23 |
| (1,23) | 1:34:A:LEU:H | 1:34:A:LEU:HG | 2 | 0.23 | 0.06 | 0.23 |
| (1,637) | 1:176:A:ASP:H | 1:183:A:VAL:H | 2 | 0.23 | 0.06 | 0.23 |
| (1,1639) | 1:19:A:ARG:H | 1:20:A:LEU:HB2 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2214) | 1:136:A:ASN:HD21 | 1:140:A:GLN:HB2 | 2 | 0.23 | 0.01 | 0.23 |
| (1,2214) | 1:136:A:ASN:HD22 | 1:140:A:GLN:HB2 | 2 | 0.23 | 0.01 | 0.23 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG11 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG12 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG13 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG21 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG22 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG23 | 2 | 0.23 | 0.06 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD11 | 1:166:A:ASN:HD21 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD11 | 1:166:A:ASN:HD22 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD12 | 1:166:A:ASN:HD21 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD12 | 1:166:A:ASN:HD22 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD13 | 1:166:A:ASN:HD21 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD13 | 1:166:A:ASN:HD22 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD21 | 1:166:A:ASN:HD21 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD21 | 1:166:A:ASN:HD22 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD22 | 1:166:A:ASN:HD21 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD22 | 1:166:A:ASN:HD22 | 2 | 0.22 | 0.01 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD23 | 1:166:A:ASN:HD21 | 2 | 0.22 | 0.01 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2251) | 1:164:A:LEU:HD23 | 1:166:A:ASN:HD22 | 2 | 0.22 | 0.01 | 0.22 |
| (1,761) | 1:49:A:LEU:H | 1:165:A:PHE:HD1 | 2 | 0.22 | 0.05 | 0.22 |
| (1,761) | 1:49:A:LEU:H | 1:165:A:PHE:HD2 | 2 | 0.22 | 0.05 | 0.22 |
| (1,269) | 1:199:A:LYS:HE2 | 1:200:A:VAL:H | 2 | 0.22 | 0.03 | 0.22 |
| (1,1761) | 1:85:A:THR:HA | 1:86:A:ILE:HB | 2 | 0.22 | 0.06 | 0.22 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD11 | 2 | 0.22 | 0.02 | 0.22 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD12 | 2 | 0.22 | 0.02 | 0.22 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD13 | 2 | 0.22 | 0.02 | 0.22 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD21 | 2 | 0.22 | 0.02 | 0.22 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD22 | 2 | 0.22 | 0.02 | 0.22 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD23 | 2 | 0.22 | 0.02 | 0.22 |
| (1,665) | 1:187:A:ALA:HB1 | 1:188:A:SER:H | 2 | 0.21 | 0.02 | 0.21 |
| (1,665) | 1:187:A:ALA:HB2 | 1:188:A:SER:H | 2 | 0.21 | 0.02 | 0.21 |
| (1,665) | 1:187:A:ALA:HB3 | 1:188:A:SER:H | 2 | 0.21 | 0.02 | 0.21 |
| (1,1257) | 1:58:A:GLN:HA | 1:61:A:ASN:HD22 | 2 | 0.21 | 0.02 | 0.21 |
| (1,1401) | 1:6:A:MET:HA | 1:7:A:GLU:HB2 | 2 | 0.21 | 0.02 | 0.21 |
| (1,1345) | 1:195:A:LYS:H | 1:195:A:LYS:HD2 | 2 | 0.2 | 0.03 | 0.2 |
| (1,1493) | 1:207:A:ARG:HA | 1:207:A:ARG:HD2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1963) | 1:49:A:LEU:HD11 | 1:201:A:CYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1963) | 1:49:A:LEU:HD12 | 1:201:A:CYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1963) | 1:49:A:LEU:HD13 | 1:201:A:CYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1963) | 1:49:A:LEU:HD21 | 1:201:A:CYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1963) | 1:49:A:LEU:HD22 | 1:201:A:CYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1963) | 1:49:A:LEU:HD23 | 1:201:A:CYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG23 | 2 | 0.2 | 0.03 | 0.2 |
| (1,190) | 1:193:A:LEU:HD11 | 1:194:A:LEU:H | 2 | 0.2 | 0.04 | 0.2 |
| (1,190) | 1:193:A:LEU:HD12 | 1:194:A:LEU:H | 2 | 0.2 | 0.04 | 0.2 |
| (1,190) | 1:193:A:LEU:HD13 | 1:194:A:LEU:H | 2 | 0.2 | 0.04 | 0.2 |
| (1,190) | 1:193:A:LEU:HD21 | 1:194:A:LEU:H | 2 | 0.2 | 0.04 | 0.2 |
| (1,190) | 1:193:A:LEU:HD22 | 1:194:A:LEU:H | 2 | 0.2 | 0.04 | 0.2 |
| (1,190) | 1:193:A:LEU:HD23 | 1:194:A:LEU:H | 2 | 0.2 | 0.04 | 0.2 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 2 | 0.2 | 0.05 | 0.2 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 2 | 0.2 | 0.05 | 0.2 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 2 | 0.2 | 0.05 | 0.2 |
| (1,2033) | 1:70:A:LEU:HD11 | 1:185:A:HIS:H | 2 | 0.2 | 0.08 | 0.2 |
| (1,2033) | 1:70:A:LEU:HD12 | 1:185:A:HIS:H | 2 | 0.2 | 0.08 | 0.2 |
| (1,2033) | 1:70:A:LEU:HD13 | 1:185:A:HIS:H | 2 | 0.2 | 0.08 | 0.2 |
| (1,2033) | 1:70:A:LEU:HD21 | 1:185:A:HIS:H | 2 | 0.2 | 0.08 | 0.2 |
| (1,2033) | 1:70:A:LEU:HD22 | 1:185:A:HIS:H | 2 | 0.2 | 0.08 | 0.2 |
| (1,2033) | 1:70:A:LEU:HD23 | 1:185:A:HIS:H | 2 | 0.2 | 0.08 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,39) | 1:27:A:ARG:H | 1:221:A:LYS:HA | 2 | 0.2 | 0.02 | 0.2 |
| (1,179) | 1:213:A:ARG:H | 1:214:A:PHE:HB2 | 2 | 0.19 | 0.06 | 0.19 |
| (1,1175) | 1:77:A:PRO:HA | 1:78:A:LYS:HD2 | 2 | 0.19 | 0.05 | 0.19 |
| (1,2058) | 1:79:A:VAL:HG11 | 1:81:A:PHE:H | 2 | 0.19 | 0.06 | 0.19 |
| (1,2058) | 1:79:A:VAL:HG12 | 1:81:A:PHE:H | 2 | 0.19 | 0.06 | 0.19 |
| (1,2058) | 1:79:A:VAL:HG13 | 1:81:A:PHE:H | 2 | 0.19 | 0.06 | 0.19 |
| (1,2058) | 1:79:A:VAL:HG21 | 1:81:A:PHE:H | 2 | 0.19 | 0.06 | 0.19 |
| (1,2058) | 1:79:A:VAL:HG22 | 1:81:A:PHE:H | 2 | 0.19 | 0.06 | 0.19 |
| (1,2058) | 1:79:A:VAL:HG23 | 1:81:A:PHE:H | 2 | 0.19 | 0.06 | 0.19 |
| (1,528) | 1:60:A:GLU:HA | 1:63:A:ARG:H | 2 | 0.18 | 0.08 | 0.18 |
| (1,2009) | 1:58:A:GLN:HB2 | 1:61:A:ASN:HD21 | 2 | 0.18 | 0.04 | 0.18 |
| (1,2009) | 1:58:A:GLN:HB2 | 1:61:A:ASN:HD22 | 2 | 0.18 | 0.04 | 0.18 |
| (1,2370) | 1:221:A:LYS:HB2 | 1:222:A:ALA:HA | 2 | 0.18 | 0.06 | 0.18 |
| (1,2322) | 1:184:A:ASN:H | 1:184:A:ASN:HD21 | 2 | 0.18 | 0.06 | 0.18 |
| (1,2322) | 1:184:A:ASN:H | 1:184:A:ASN:HD22 | 2 | 0.18 | 0.06 | 0.18 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD11 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD12 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD13 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD21 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD22 | 2 | 0.18 | 0.03 | 0.18 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD23 | 2 | 0.18 | 0.03 | 0.18 |
| (1,2067) | 1:79:A:VAL:HG11 | 1:173:A:TYR:HA | 2 | 0.17 | 0.06 | 0.17 |
| (1,2067) | 1:79:A:VAL:HG12 | 1:173:A:TYR:HA | 2 | 0.17 | 0.06 | 0.17 |
| (1,2067) | 1:79:A:VAL:HG13 | 1:173:A:TYR:HA | 2 | 0.17 | 0.06 | 0.17 |
| (1,2067) | 1:79:A:VAL:HG21 | 1:173:A:TYR:HA | 2 | 0.17 | 0.06 | 0.17 |
| (1,2067) | 1:79:A:VAL:HG22 | 1:173:A:TYR:HA | 2 | 0.17 | 0.06 | 0.17 |
| (1,2067) | 1:79:A:VAL:HG23 | 1:173:A:TYR:HA | 2 | 0.17 | 0.06 | 0.17 |
| (1,1793) | 1:18:A:TYR:HD1 | 1:21:A:GLY:HA2 | 2 | 0.16 | 0.01 | 0.16 |
| (1,1793) | 1:18:A:TYR:HD2 | 1:21:A:GLY:HA2 | 2 | 0.16 | 0.01 | 0.16 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG11 | 2 | 0.16 | 0.04 | 0.16 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG12 | 2 | 0.16 | 0.04 | 0.16 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG13 | 2 | 0.16 | 0.04 | 0.16 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG21 | 2 | 0.16 | 0.04 | 0.16 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG22 | 2 | 0.16 | 0.04 | 0.16 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG23 | 2 | 0.16 | 0.04 | 0.16 |
| (1,454) | 1:112:A:SER:H | 1:115:A:LYS:HB2 | 2 | 0.16 | 0.05 | 0.16 |
| (1,657) | 1:42:A:VAL:H | 1:42:A:VAL:HB | 2 | 0.16 | 0.01 | 0.16 |
| (1,1117) | 1:197:A:ALA:HA | 1:201:A:CYS:HB2 | 2 | 0.16 | 0.03 | 0.16 |
| (1,1284) | 1:80:A:TYR:HD1 | 1:100:A:ALA:HA | 2 | 0.16 | 0.04 | 0.16 |
| (1,1284) | 1:80:A:TYR:HD2 | 1:100:A:ALA:HA | 2 | 0.16 | 0.04 | 0.16 |
| (1,1788) | 1:14:A:ASN:HB2 | 1:18:A:TYR:HE1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1788) | 1:14:A:ASN:HB2 | 1:18:A:TYR:HE2 | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2181) | 1:122:A:GLU:HB2 | 1:123:A:LYS:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,2232) | 1:151:A:GLN:HB2 | 1:151:A:GLN:HE21 | 2 | 0.16 | 0.02 | 0.16 |
| (1,2232) | 1:151:A:GLN:HB2 | 1:151:A:GLN:HE22 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1814) | 1:3:A:LEU:HD11 | 1:143:A:HIS:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1814) | 1:3:A:LEU:HD12 | 1:143:A:HIS:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1814) | 1:3:A:LEU:HD13 | 1:143:A:HIS:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1814) | 1:3:A:LEU:HD21 | 1:143:A:HIS:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1814) | 1:3:A:LEU:HD22 | 1:143:A:HIS:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1814) | 1:3:A:LEU:HD23 | 1:143:A:HIS:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,704) | 1:23:A:ALA:HA | 1:25:A:GLN:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,1199) | 1:5:A:PRO:HA | 1:88:A:ASN:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB1 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB2 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB3 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD21 | 2 | 0.16 | 0.01 | 0.16 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD22 | 2 | 0.16 | 0.01 | 0.16 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD23 | 2 | 0.16 | 0.01 | 0.16 |
| (1,726) | 1:99:A:VAL:HB | 1:100:A:ALA:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,999) | 1:15:A:LYS:H | 1:16:A:VAL:HA | 2 | 0.15 | 0.02 | 0.15 |
| (1,1541) | 1:112:A:SER:HA | 1:113:A:VAL:HB | 2 | 0.15 | 0.03 | 0.15 |
| (1,62) | 1:38:A:SER:HA | 1:40:A:GLY:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,604) | 1:124:A:MET:H | 1:125:A:SER:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,1163) | 1:92:A:THR:HB | 1:93:A:ILE:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1543) | 1:144:A:ASP:HA | 1:146:A:VAL:H | 2 | 0.14 | 0.01 | 0.14 |
| (1,1204) | 1:75:A:VAL:HG11 | 1:76:A:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1204) | 1:75:A:VAL:HG12 | 1:76:A:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1204) | 1:75:A:VAL:HG13 | 1:76:A:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1204) | 1:75:A:VAL:HG21 | 1:76:A:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1204) | 1:75:A:VAL:HG22 | 1:76:A:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1204) | 1:75:A:VAL:HG23 | 1:76:A:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1481) | 1:121:A:THR:HG21 | 1:124:A:MET:HG2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1481) | 1:121:A:THR:HG22 | 1:124:A:MET:HG2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1481) | 1:121:A:THR:HG23 | 1:124:A:MET:HG2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1927) | 1:36:A:GLU:H | 1:36:A:GLU:HG2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1932) | 1:36:A:GLU:HG2 | 1:37:A:GLU:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,520) | 1:17:A:LEU:H | 1:19:A:ARG:H | 2 | 0.13 | 0.03 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD11 | 2 | 0.13 | 0.0 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD12 | 2 | 0.13 | 0.0 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD13 | 2 | 0.13 | 0.0 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD23 | 2 | 0.13 | 0.0 | 0.13 |

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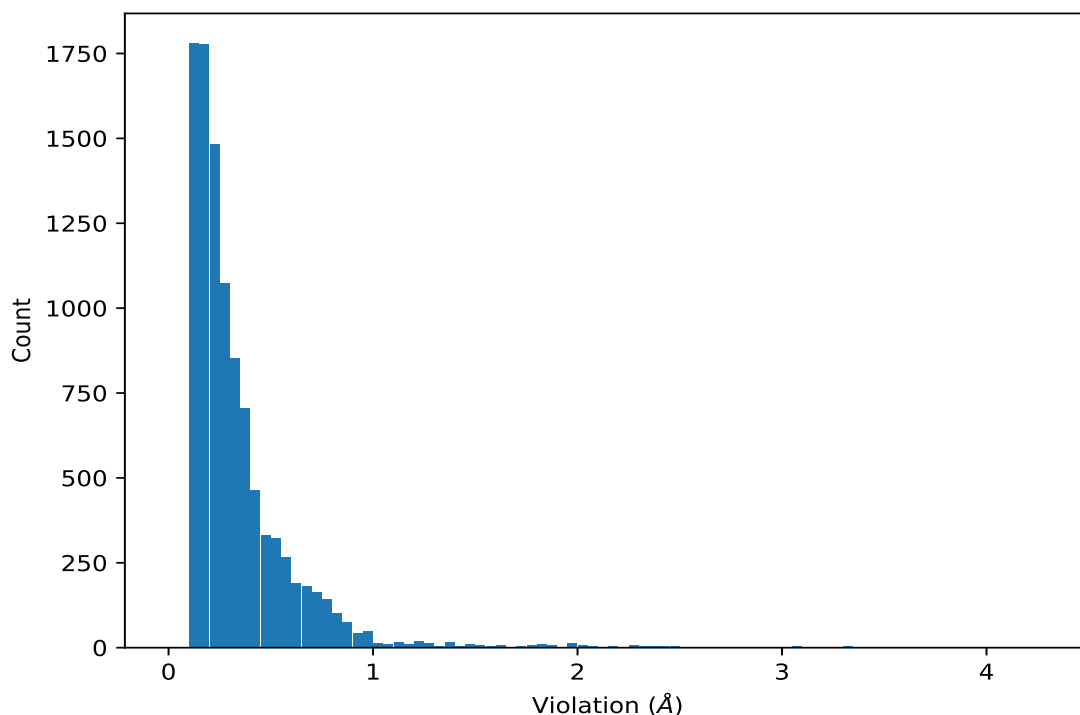
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1629) | 1:131:A:LYS:HA | 1:135:A:LYS:HG2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,603) | 1:14:A:ASN:H | 1:28:A:PHE:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 2 | 0.12 | 0.02 | 0.12 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 2 | 0.12 | 0.02 | 0.12 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 2 | 0.12 | 0.02 | 0.12 |
| (1,939) | 1:98:A:ALA:HA | 1:101:A:ASN:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG11 | 2 | 0.12 | 0.01 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG13 | 2 | 0.12 | 0.01 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG21 | 2 | 0.12 | 0.01 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG22 | 2 | 0.12 | 0.01 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG23 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD11 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD12 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD13 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1366) | 1:117:A:PHE:H | 1:118:A:LEU:HA | 2 | 0.12 | 0.02 | 0.12 |
| (1,457) | 1:152:A:CYS:HA | 1:153:A:ARG:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,497) | 1:49:A:LEU:HA | 1:217:A:VAL:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,1348) | 1:157:A:LYS:H | 1:157:A:LYS:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2271) | 1:167:A:ASN:HB2 | 1:170:A:GLY:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,1262) | 1:156:A:ASP:HA | 1:157:A:LYS:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,247) | 1:166:A:ASN:H | 1:174:A:GLU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG11 | 2 | 0.11 | 0.01 | 0.11 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG12 | 2 | 0.11 | 0.01 | 0.11 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG13 | 2 | 0.11 | 0.01 | 0.11 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG21 | 2 | 0.11 | 0.01 | 0.11 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG22 | 2 | 0.11 | 0.01 | 0.11 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG23 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1154) | 1:30:A:ASP:HB2 | 1:217:A:VAL:HA | 2 | 0.11 | 0.01 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 14 | 4.28 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 9 | 4.17 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 17 | 4.11 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 2 | 4.1 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 10 | 4.08 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 3 | 3.96 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 20 | 3.94 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 11 | 3.92 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 1 | 3.89 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 1 | 3.85 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 7 | 3.77 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 16 | 3.76 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 12 | 3.73 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 15 | 3.65 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 6 | 3.6 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 14 | 3.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 5 | 3.57 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 19 | 3.55 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 14 | 3.45 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 17 | 3.4 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 4 | 3.34 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 7 | 3.31 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 8 | 3.3 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 9 | 3.25 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 18 | 3.2 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 14 | 3.05 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 14 | 3.05 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 14 | 3.05 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 2 | 3.03 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 14 | 2.97 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 10 | 2.93 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 17 | 2.84 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 20 | 2.67 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 16 | 2.64 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 12 | 2.58 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 7 | 2.49 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 7 | 2.49 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 7 | 2.49 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 1 | 2.45 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 11 | 2.43 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 2 | 2.43 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 7 | 2.41 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 3 | 2.39 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 9 | 2.38 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 20 | 2.35 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 1 | 2.34 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 1 | 2.34 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 1 | 2.34 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 10 | 2.34 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 17 | 2.33 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 11 | 2.28 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 3 | 2.27 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 17 | 2.26 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 17 | 2.26 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 17 | 2.26 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 1 | 2.26 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 2 | 2.23 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 8 | 2.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 7 | 2.18 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 19 | 2.17 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 6 | 2.15 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 16 | 2.12 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 12 | 2.1 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 5 | 2.08 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 9 | 2.08 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 15 | 2.06 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 20 | 2.02 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 20 | 2.02 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 20 | 2.02 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 20 | 2.02 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 20 | 2.02 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 20 | 2.02 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 19 | 1.98 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 19 | 1.98 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 19 | 1.98 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 19 | 1.98 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 19 | 1.98 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 19 | 1.98 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 3 | 1.97 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 3 | 1.97 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 3 | 1.97 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 3 | 1.97 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 3 | 1.97 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 3 | 1.97 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 18 | 1.96 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 6 | 1.86 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 6 | 1.86 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 6 | 1.86 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 6 | 1.86 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 6 | 1.86 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 6 | 1.86 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 4 | 1.85 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 10 | 1.84 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 6 | 1.83 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 3 | 1.83 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 16 | 1.82 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 16 | 1.82 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 16 | 1.82 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 16 | 1.82 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 16 | 1.82 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 16 | 1.82 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 16 | 1.8 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 10 | 1.79 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 10 | 1.79 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 10 | 1.79 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 5 | 1.79 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 8 | 1.77 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE21 | 1 | 1.76 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE22 | 1 | 1.76 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 15 | 1.76 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 9 | 1.71 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 9 | 1.71 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 9 | 1.71 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 4 | 1.68 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 2 | 1.64 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 2 | 1.64 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 2 | 1.64 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 16 | 1.61 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 16 | 1.61 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 16 | 1.61 |
| (1,1749) | 1:80:A:TYR:HE1 | 1:121:A:THR:HB | 19 | 1.61 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 8 | 1.59 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 12 | 1.56 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 12 | 1.56 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 12 | 1.56 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 2 | 1.52 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 2 | 1.52 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 2 | 1.52 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 2 | 1.52 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 2 | 1.52 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 2 | 1.52 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 7 | 1.49 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 11 | 1.48 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 5 | 1.45 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 5 | 1.45 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 5 | 1.45 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 5 | 1.45 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 5 | 1.45 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 5 | 1.45 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 5 | 1.45 |
| (1,609) | 1:80:A:TYR:HE1 | 1:122:A:GLU:H | 18 | 1.45 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 11 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 11 | 1.41 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 11 | 1.41 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 1 | 1.39 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 1 | 1.39 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 3 | 1.39 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 3 | 1.39 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 3 | 1.39 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 8 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 8 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 8 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 8 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 8 | 1.38 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 8 | 1.38 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 12 | 1.38 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 15 | 1.37 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 15 | 1.37 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 15 | 1.37 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 2 | 1.33 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 8 | 1.33 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 19 | 1.3 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 11 | 1.29 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 11 | 1.29 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 3 | 1.27 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 3 | 1.27 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 3 | 1.27 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 9 | 1.27 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 9 | 1.27 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 9 | 1.27 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 9 | 1.27 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 4 | 1.26 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 4 | 1.26 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 20 | 1.25 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 20 | 1.25 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 20 | 1.25 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 5 | 1.24 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 5 | 1.24 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 6 | 1.24 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 6 | 1.24 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 6 | 1.24 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 19 | 1.24 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 19 | 1.24 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 19 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2126) | 1:104:A:ASP:H | 1:105:A:LYS:HE2 | 2 | 1.23 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 15 | 1.23 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 15 | 1.23 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 8 | 1.23 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 8 | 1.23 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 8 | 1.23 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 20 | 1.23 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 20 | 1.23 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 20 | 1.23 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 4 | 1.22 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 6 | 1.21 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 8 | 1.16 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 8 | 1.16 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 14 | 1.16 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 10 | 1.16 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 10 | 1.16 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 10 | 1.16 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 5 | 1.16 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 7 | 1.15 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 15 | 1.15 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 11 | 1.14 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 11 | 1.14 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 11 | 1.14 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE21 | 13 | 1.13 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE22 | 13 | 1.13 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 8 | 1.13 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 8 | 1.13 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 20 | 1.13 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 7 | 1.1 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 7 | 1.1 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 7 | 1.1 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 7 | 1.1 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 7 | 1.1 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 7 | 1.1 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 18 | 1.1 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 18 | 1.1 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 18 | 1.1 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 13 | 1.08 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 13 | 1.08 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 15 | 1.07 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 15 | 1.07 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 15 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 9 | 1.05 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 9 | 1.05 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 9 | 1.05 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 9 | 1.05 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 9 | 1.05 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 9 | 1.05 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 18 | 1.04 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 18 | 1.04 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 18 | 1.04 |
| (1,2179) | 1:121:A:THR:HG21 | 1:124:A:MET:HB2 | 9 | 1.02 |
| (1,2179) | 1:121:A:THR:HG22 | 1:124:A:MET:HB2 | 9 | 1.02 |
| (1,2179) | 1:121:A:THR:HG23 | 1:124:A:MET:HB2 | 9 | 1.02 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 4 | 1.02 |
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 1 | 1.0 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 1 | 1.0 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 4 | 1.0 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 4 | 1.0 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 4 | 1.0 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 4 | 0.99 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 4 | 0.99 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 4 | 0.99 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 16 | 0.99 |
| (1,2178) | 1:121:A:THR:HB | 1:124:A:MET:HB2 | 9 | 0.98 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 2 | 0.98 |
| (1,1574) | 1:166:A:ASN:H | 1:175:A:LEU:HG | 18 | 0.98 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE1 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE2 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE3 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE1 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE2 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE3 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE1 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE2 | 6 | 0.97 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE3 | 6 | 0.97 |
| (1,974) | 1:82:A:MET:HE1 | 1:92:A:THR:HB | 5 | 0.97 |
| (1,974) | 1:82:A:MET:HE2 | 1:92:A:THR:HB | 5 | 0.97 |
| (1,974) | 1:82:A:MET:HE3 | 1:92:A:THR:HB | 5 | 0.97 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 9 | 0.97 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 9 | 0.97 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 9 | 0.97 |
| (1,2015) | 1:61:A:ASN:HD21 | 1:62:A:PHE:H | 4 | 0.96 |
| (1,2015) | 1:61:A:ASN:HD22 | 1:62:A:PHE:H | 4 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 1 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 1 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 1 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 1 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 1 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 1 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 5 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 5 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 5 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 5 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 5 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 5 | 0.95 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 10 | 0.95 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 10 | 0.95 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 10 | 0.95 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 10 | 0.95 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 10 | 0.95 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 10 | 0.95 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 16 | 0.95 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 16 | 0.95 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 16 | 0.95 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG21 | 17 | 0.95 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG22 | 17 | 0.95 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG23 | 17 | 0.95 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 20 | 0.95 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 16 | 0.94 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 16 | 0.94 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 16 | 0.94 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 16 | 0.94 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 16 | 0.94 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 16 | 0.94 |
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 16 | 0.94 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 16 | 0.94 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 14 | 0.93 |
| (1,1732) | 1:122:A:GLU:HG2 | 1:123:A:LYS:HG2 | 8 | 0.93 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 7 | 0.93 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 13 | 0.92 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 13 | 0.92 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 13 | 0.92 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 13 | 0.92 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 13 | 0.92 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 13 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 11 | 0.92 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 9 | 0.92 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 15 | 0.92 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 15 | 0.92 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 15 | 0.92 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 9 | 0.91 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 9 | 0.91 |
| (1,2015) | 1:61:A:ASN:HD21 | 1:62:A:PHE:H | 8 | 0.91 |
| (1,2015) | 1:61:A:ASN:HD22 | 1:62:A:PHE:H | 8 | 0.91 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 1 | 0.91 |
| (1,1574) | 1:166:A:ASN:H | 1:175:A:LEU:HG | 6 | 0.91 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 6 | 0.91 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 19 | 0.91 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 18 | 0.91 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 1 | 0.91 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 5 | 0.91 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 5 | 0.91 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 5 | 0.91 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 13 | 0.9 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 13 | 0.9 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 13 | 0.9 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 13 | 0.9 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 13 | 0.9 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 13 | 0.9 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 2 | 0.9 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 1 | 0.9 |
| (1,2015) | 1:61:A:ASN:HD21 | 1:62:A:PHE:H | 15 | 0.89 |
| (1,2015) | 1:61:A:ASN:HD22 | 1:62:A:PHE:H | 15 | 0.89 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 7 | 0.89 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 7 | 0.89 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 7 | 0.89 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 7 | 0.89 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 7 | 0.89 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 7 | 0.89 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 9 | 0.88 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 9 | 0.88 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 9 | 0.88 |
| (1,1051) | 1:23:A:ALA:HB1 | 1:107:A:GLY:H | 9 | 0.88 |
| (1,1051) | 1:23:A:ALA:HB2 | 1:107:A:GLY:H | 9 | 0.88 |
| (1,1051) | 1:23:A:ALA:HB3 | 1:107:A:GLY:H | 9 | 0.88 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 6 | 0.88 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 6 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 6 | 0.88 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 5 | 0.88 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 18 | 0.88 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 11 | 0.87 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 11 | 0.87 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 11 | 0.87 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 11 | 0.87 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 11 | 0.87 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 11 | 0.87 |
| (1,2015) | 1:61:A:ASN:HD21 | 1:62:A:PHE:H | 11 | 0.87 |
| (1,2015) | 1:61:A:ASN:HD22 | 1:62:A:PHE:H | 11 | 0.87 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 5 | 0.87 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 5 | 0.87 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 5 | 0.87 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 11 | 0.87 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 19 | 0.86 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 19 | 0.86 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 19 | 0.86 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 19 | 0.86 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 19 | 0.86 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 19 | 0.86 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 8 | 0.86 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 8 | 0.86 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 8 | 0.86 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 8 | 0.86 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 8 | 0.86 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 8 | 0.86 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 8 | 0.86 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 8 | 0.86 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 8 | 0.86 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 1 | 0.86 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 1 | 0.86 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 1 | 0.86 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 1 | 0.86 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 1 | 0.86 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 1 | 0.86 |
| (1,1574) | 1:166:A:ASN:H | 1:175:A:LEU:HG | 4 | 0.86 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE21 | 13 | 0.85 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE22 | 13 | 0.85 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 3 | 0.85 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 3 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 2 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 2 | 0.85 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 2 | 0.85 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 7 | 0.85 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 7 | 0.85 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 7 | 0.85 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 15 | 0.85 |
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 15 | 0.85 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 15 | 0.85 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 9 | 0.85 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 9 | 0.85 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 6 | 0.84 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 6 | 0.84 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 6 | 0.84 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 6 | 0.84 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 6 | 0.84 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 6 | 0.84 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 5 | 0.84 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 15 | 0.84 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 7 | 0.84 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 7 | 0.84 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 8 | 0.84 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 8 | 0.84 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 19 | 0.84 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 4 | 0.84 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 4 | 0.84 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 4 | 0.84 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 10 | 0.83 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 10 | 0.83 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 10 | 0.83 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 10 | 0.83 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 10 | 0.83 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 10 | 0.83 |
| (1,2189) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 6 | 0.83 |
| (1,2189) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 6 | 0.83 |
| (1,2189) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 6 | 0.83 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 14 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1211) | 1:52:A:LEU:HA | 1:215:A:SER:HB2 | 6 | 0.83 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 13 | 0.83 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 16 | 0.83 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 16 | 0.83 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 16 | 0.83 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 16 | 0.83 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 16 | 0.83 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 16 | 0.83 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 16 | 0.82 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 16 | 0.82 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 10 | 0.82 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 10 | 0.82 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 10 | 0.82 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 3 | 0.82 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 3 | 0.82 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 12 | 0.82 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 12 | 0.82 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 12 | 0.82 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 3 | 0.82 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 20 | 0.82 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 15 | 0.82 |
| (1,1191) | 1:37:A:GLU:HG2 | 1:38:A:SER:HB2 | 7 | 0.82 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 4 | 0.82 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 4 | 0.82 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 4 | 0.82 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE1 | 18 | 0.82 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE2 | 18 | 0.82 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE3 | 18 | 0.82 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 17 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 17 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 17 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 17 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 17 | 0.81 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 17 | 0.81 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE21 | 9 | 0.81 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE22 | 9 | 0.81 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 1 | 0.81 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 1 | 0.81 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 1 | 0.81 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 10 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 14 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 14 | 0.81 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 14 | 0.81 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 5 | 0.81 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 5 | 0.81 |
| (1,2210) | 1:136:A:ASN:HD21 | 1:137:A:GLU:HB2 | 19 | 0.8 |
| (1,2210) | 1:136:A:ASN:HD22 | 1:137:A:GLU:HB2 | 19 | 0.8 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 2 | 0.8 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 2 | 0.8 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 19 | 0.8 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 19 | 0.8 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 19 | 0.8 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 19 | 0.8 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 19 | 0.8 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 19 | 0.8 |
| (1,1732) | 1:122:A:GLU:HG2 | 1:123:A:LYS:HG2 | 9 | 0.8 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE1 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE2 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE3 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE1 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE2 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE3 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE1 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE2 | 8 | 0.8 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE3 | 8 | 0.8 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 12 | 0.8 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 16 | 0.8 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 16 | 0.8 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD1 | 14 | 0.8 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD2 | 14 | 0.8 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 5 | 0.8 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 5 | 0.79 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 5 | 0.79 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 5 | 0.79 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 5 | 0.79 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 5 | 0.79 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 5 | 0.79 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 6 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 5 | 0.79 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 5 | 0.79 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 5 | 0.79 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 5 | 0.79 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 5 | 0.79 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 5 | 0.79 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 18 | 0.79 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 20 | 0.78 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 20 | 0.78 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 20 | 0.78 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 20 | 0.78 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 20 | 0.78 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 20 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 2 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 2 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 2 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 2 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 2 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 2 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 3 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 3 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 3 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 3 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 3 | 0.78 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 3 | 0.78 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 9 | 0.78 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE1 | 6 | 0.78 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE2 | 6 | 0.78 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE3 | 6 | 0.78 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 5 | 0.78 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 5 | 0.78 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 5 | 0.78 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 12 | 0.78 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 18 | 0.78 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 18 | 0.78 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE1 | 16 | 0.78 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE2 | 16 | 0.78 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE3 | 16 | 0.78 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 5 | 0.78 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 5 | 0.78 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 5 | 0.78 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 7 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 7 | 0.78 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 7 | 0.78 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 15 | 0.78 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 15 | 0.78 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 11 | 0.77 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 11 | 0.77 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 11 | 0.77 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 11 | 0.77 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 11 | 0.77 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 11 | 0.77 |
| (1,2098) | 1:99:A:VAL:HA | 1:102:A:ASN:HD21 | 9 | 0.77 |
| (1,2098) | 1:99:A:VAL:HA | 1:102:A:ASN:HD22 | 9 | 0.77 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 8 | 0.77 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 8 | 0.77 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 8 | 0.77 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 8 | 0.77 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 8 | 0.77 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 8 | 0.77 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 18 | 0.77 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 11 | 0.77 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 2 | 0.77 |
| (1,968) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 6 | 0.77 |
| (1,968) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 6 | 0.77 |
| (1,968) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 6 | 0.77 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 1 | 0.77 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 1 | 0.77 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 1 | 0.77 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 1 | 0.77 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 1 | 0.77 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 1 | 0.77 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 14 | 0.77 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 14 | 0.77 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 14 | 0.77 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 14 | 0.77 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 14 | 0.77 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 14 | 0.77 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 20 | 0.76 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 20 | 0.76 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 20 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 14 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 14 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 14 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 14 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 14 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 14 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 15 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 15 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 15 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 15 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 15 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 15 | 0.76 |
| (1,2199) | 1:135:A:LYS:H | 1:140:A:GLN:HE21 | 10 | 0.76 |
| (1,2199) | 1:135:A:LYS:H | 1:140:A:GLN:HE22 | 10 | 0.76 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 4 | 0.76 |
| (1,1885) | 1:25:A:GLN:HE21 | 1:26:A:TRP:H | 11 | 0.76 |
| (1,1885) | 1:25:A:GLN:HE22 | 1:26:A:TRP:H | 11 | 0.76 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 14 | 0.76 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 8 | 0.76 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 8 | 0.76 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 8 | 0.76 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 10 | 0.76 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 9 | 0.75 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 9 | 0.75 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 9 | 0.75 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 9 | 0.75 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 9 | 0.75 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 9 | 0.75 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 16 | 0.75 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 16 | 0.75 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 16 | 0.75 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 9 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD21 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD22 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD23 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD21 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD22 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD23 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD21 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD22 | 10 | 0.75 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD23 | 10 | 0.75 |
| (1,1398) | 1:81:A:PHE:H | 1:82:A:MET:HA | 12 | 0.75 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 9 | 0.75 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 9 | 0.75 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 9 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 10 | 0.75 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 10 | 0.75 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 10 | 0.75 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 13 | 0.75 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 13 | 0.75 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 13 | 0.75 |
| (1,669) | 1:189:A:SER:H | 1:193:A:LEU:H | 7 | 0.75 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 9 | 0.75 |
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 9 | 0.75 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 9 | 0.75 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 6 | 0.74 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 6 | 0.74 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 6 | 0.74 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 6 | 0.74 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 6 | 0.74 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 6 | 0.74 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 3 | 0.74 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 3 | 0.74 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 3 | 0.74 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 14 | 0.74 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 14 | 0.74 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 14 | 0.74 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 5 | 0.74 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 10 | 0.74 |
| (1,1886) | 1:25:A:GLN:HE21 | 1:221:A:LYS:HE2 | 13 | 0.74 |
| (1,1886) | 1:25:A:GLN:HE22 | 1:221:A:LYS:HE2 | 13 | 0.74 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 8 | 0.74 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 8 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 4 | 0.74 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 4 | 0.74 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD1 | 5 | 0.74 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD2 | 5 | 0.74 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD1 | 17 | 0.74 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD2 | 17 | 0.74 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 4 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 2 | 0.73 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 2 | 0.73 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 2 | 0.73 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 2 | 0.73 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 2 | 0.73 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 2 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 7 | 0.73 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 7 | 0.73 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 15 | 0.73 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 15 | 0.73 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 15 | 0.73 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 14 | 0.73 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 14 | 0.73 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 14 | 0.73 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 14 | 0.73 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 14 | 0.73 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 14 | 0.73 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 3 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 10 | 0.73 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 10 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 10 | 0.73 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 9 | 0.73 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 9 | 0.73 |
| (1,1051) | 1:23:A:ALA:HB1 | 1:107:A:GLY:H | 12 | 0.73 |
| (1,1051) | 1:23:A:ALA:HB2 | 1:107:A:GLY:H | 12 | 0.73 |
| (1,1051) | 1:23:A:ALA:HB3 | 1:107:A:GLY:H | 12 | 0.73 |
| (1,293) | 1:52:A:LEU:HG | 1:53:A:PHE:H | 5 | 0.73 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 9 | 0.72 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 9 | 0.72 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 2 | 0.72 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 2 | 0.72 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 2 | 0.72 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 8 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 7 | 0.72 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 7 | 0.72 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 7 | 0.72 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 7 | 0.72 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 10 | 0.72 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 10 | 0.72 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 15 | 0.72 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 1 | 0.72 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 1 | 0.72 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 19 | 0.72 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 19 | 0.72 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD11 | 13 | 0.71 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD12 | 13 | 0.71 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD13 | 13 | 0.71 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD21 | 13 | 0.71 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD22 | 13 | 0.71 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD23 | 13 | 0.71 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 6 | 0.71 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 3 | 0.71 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 3 | 0.71 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 3 | 0.71 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 3 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 3 | 0.71 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 3 | 0.71 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 19 | 0.71 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 19 | 0.71 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 19 | 0.71 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG21 | 19 | 0.71 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG22 | 19 | 0.71 |
| (1,1785) | 1:80:A:TYR:HE1 | 1:121:A:THR:HG23 | 19 | 0.71 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 6 | 0.71 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 6 | 0.71 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 6 | 0.71 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 5 | 0.71 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 18 | 0.71 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 13 | 0.71 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 1 | 0.71 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 1 | 0.71 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 1 | 0.71 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 1 | 0.71 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 14 | 0.71 |
| (1,2) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 5 | 0.71 |
| (1,2) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 5 | 0.71 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 6 | 0.7 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 6 | 0.7 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 5 | 0.7 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 5 | 0.7 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 5 | 0.7 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 5 | 0.7 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 5 | 0.7 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 5 | 0.7 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 5 | 0.7 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 8 | 0.7 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 8 | 0.7 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 8 | 0.7 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 5 | 0.7 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 4 | 0.7 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 5 | 0.7 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 9 | 0.7 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 16 | 0.7 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 20 | 0.7 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 20 | 0.7 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 20 | 0.7 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 14 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 14 | 0.7 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 14 | 0.7 |
| (1,737) | 1:164:A:LEU:H | 1:177:A:GLY:H | 9 | 0.7 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 5 | 0.7 |
| (1,1) | 1:167:A:ASN:HD22 | 1:190:A:GLU:HA | 9 | 0.7 |
| (1,2284) | 1:167:A:ASN:HD21 | 1:193:A:LEU:HA | 19 | 0.69 |
| (1,2284) | 1:167:A:ASN:HD22 | 1:193:A:LEU:HA | 19 | 0.69 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 2 | 0.69 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 2 | 0.69 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 3 | 0.69 |
| (1,1574) | 1:166:A:ASN:H | 1:175:A:LEU:HG | 3 | 0.69 |
| (1,1574) | 1:166:A:ASN:H | 1:175:A:LEU:HG | 8 | 0.69 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 7 | 0.69 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 17 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 15 | 0.69 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 15 | 0.69 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 16 | 0.69 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 13 | 0.69 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 13 | 0.69 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 12 | 0.69 |
| (1,801) | 1:56:A:THR:HG21 | 1:57:A:ALA:HA | 7 | 0.69 |
| (1,801) | 1:56:A:THR:HG22 | 1:57:A:ALA:HA | 7 | 0.69 |
| (1,801) | 1:56:A:THR:HG23 | 1:57:A:ALA:HA | 7 | 0.69 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 5 | 0.69 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 5 | 0.69 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 5 | 0.69 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 14 | 0.69 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 14 | 0.69 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 14 | 0.69 |
| (1,113) | 1:85:A:THR:HA | 1:87:A:GLY:H | 8 | 0.69 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 5 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 5 | 0.68 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 5 | 0.68 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE21 | 1 | 0.68 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE22 | 1 | 0.68 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE21 | 17 | 0.68 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE22 | 17 | 0.68 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 19 | 0.68 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 7 | 0.68 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 7 | 0.68 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 7 | 0.68 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 7 | 0.68 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 7 | 0.68 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 7 | 0.68 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 12 | 0.68 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 20 | 0.68 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 4 | 0.68 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 4 | 0.68 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 4 | 0.68 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 6 | 0.68 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 12 | 0.68 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 12 | 0.68 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 20 | 0.68 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 20 | 0.68 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 19 | 0.68 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 19 | 0.68 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 19 | 0.68 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 16 | 0.68 |
| (1,434) | 1:121:A:THR:HG21 | 1:129:A:ARG:H | 9 | 0.68 |
| (1,434) | 1:121:A:THR:HG22 | 1:129:A:ARG:H | 9 | 0.68 |
| (1,434) | 1:121:A:THR:HG23 | 1:129:A:ARG:H | 9 | 0.68 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 12 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 12 | 0.68 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 12 | 0.68 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 12 | 0.68 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 12 | 0.68 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 12 | 0.68 |
| (1,2189) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 8 | 0.67 |
| (1,2189) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 8 | 0.67 |
| (1,2189) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 8 | 0.67 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 19 | 0.67 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 19 | 0.67 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 19 | 0.67 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 19 | 0.67 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 19 | 0.67 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 19 | 0.67 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 7 | 0.67 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 7 | 0.67 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 7 | 0.67 |
| (1,1410) | 1:137:A:GLU:H | 1:140:A:GLN:HB2 | 5 | 0.67 |
| (1,1188) | 1:36:A:GLU:H | 1:38:A:SER:HB2 | 1 | 0.67 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 8 | 0.67 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 8 | 0.67 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 8 | 0.67 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 4 | 0.67 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 8 | 0.67 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 4 | 0.67 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 5 | 0.67 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 5 | 0.67 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 5 | 0.67 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 17 | 0.67 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 5 | 0.66 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 5 | 0.66 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 5 | 0.66 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 20 | 0.66 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 20 | 0.66 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 20 | 0.66 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 16 | 0.66 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 16 | 0.66 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 16 | 0.66 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 13 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 5 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 5 | 0.66 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 5 | 0.66 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 7 | 0.66 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 7 | 0.66 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 17 | 0.66 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 17 | 0.66 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 19 | 0.66 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 4 | 0.66 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 1 | 0.66 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 1 | 0.66 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD11 | 12 | 0.65 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD12 | 12 | 0.65 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD13 | 12 | 0.65 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD21 | 12 | 0.65 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD22 | 12 | 0.65 |
| (1,2261) | 1:166:A:ASN:H | 1:175:A:LEU:HD23 | 12 | 0.65 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 16 | 0.65 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 16 | 0.65 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 16 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 1 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 1 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 1 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 1 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 1 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 1 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 9 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 9 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 9 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 9 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 9 | 0.65 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 9 | 0.65 |
| (1,1717) | 1:118:A:LEU:H | 1:120:A:GLU:HG2 | 9 | 0.65 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 12 | 0.65 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 17 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 4 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 4 | 0.65 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 4 | 0.65 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD11 | 9 | 0.65 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD12 | 9 | 0.65 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD13 | 9 | 0.65 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 7 | 0.65 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 7 | 0.65 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 7 | 0.65 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 6 | 0.65 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 6 | 0.65 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 6 | 0.65 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 6 | 0.65 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 6 | 0.65 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 6 | 0.65 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 5 | 0.65 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 12 | 0.65 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 10 | 0.64 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 10 | 0.64 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 10 | 0.64 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 10 | 0.64 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 10 | 0.64 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 10 | 0.64 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE21 | 19 | 0.64 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE22 | 19 | 0.64 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 6 | 0.64 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 6 | 0.64 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 6 | 0.64 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 6 | 0.64 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 19 | 0.64 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 19 | 0.64 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 19 | 0.64 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 19 | 0.64 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 19 | 0.64 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 19 | 0.64 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 20 | 0.64 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 20 | 0.64 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 20 | 0.64 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 20 | 0.64 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 20 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 20 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB1 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB2 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB3 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB1 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB2 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB3 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB1 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB2 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB3 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB1 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB2 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB3 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB1 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB2 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB3 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB1 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB2 | 1 | 0.64 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB3 | 1 | 0.64 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 4 | 0.64 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 14 | 0.64 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 5 | 0.64 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 5 | 0.64 |
| (1,1003) | 1:131:A:LYS:HA | 1:134:A:GLU:HB2 | 1 | 0.64 |
| (1,971) | 1:12:A:MET:HE1 | 1:150:A:GLY:H | 4 | 0.64 |
| (1,971) | 1:12:A:MET:HE2 | 1:150:A:GLY:H | 4 | 0.64 |
| (1,971) | 1:12:A:MET:HE3 | 1:150:A:GLY:H | 4 | 0.64 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 2 | 0.64 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 2 | 0.64 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 2 | 0.64 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 2 | 0.63 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 2 | 0.63 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 2 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD21 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD22 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD21 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD22 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD21 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD22 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD21 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD22 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD21 | 9 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD22 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD21 | 9 | 0.63 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD22 | 9 | 0.63 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 16 | 0.63 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 16 | 0.63 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 16 | 0.63 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 16 | 0.63 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 16 | 0.63 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 16 | 0.63 |
| (1,1519) | 1:16:A:VAL:HB | 1:95:A:LEU:HB2 | 20 | 0.63 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 1 | 0.63 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 12 | 0.63 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 17 | 0.63 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 9 | 0.63 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 16 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 14 | 0.63 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 14 | 0.63 |
| (1,962) | 1:124:A:MET:HE1 | 1:129:A:ARG:H | 6 | 0.63 |
| (1,962) | 1:124:A:MET:HE2 | 1:129:A:ARG:H | 6 | 0.63 |
| (1,962) | 1:124:A:MET:HE3 | 1:129:A:ARG:H | 6 | 0.63 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 7 | 0.63 |
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 7 | 0.63 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 7 | 0.63 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 2 | 0.63 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 2 | 0.63 |
| (1,80) | 1:52:A:LEU:H | 1:53:A:PHE:HD1 | 7 | 0.63 |
| (1,80) | 1:52:A:LEU:H | 1:53:A:PHE:HD2 | 7 | 0.63 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 18 | 0.62 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 18 | 0.62 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 18 | 0.62 |
| (1,2264) | 1:166:A:ASN:HD21 | 1:175:A:LEU:H | 13 | 0.62 |
| (1,2264) | 1:166:A:ASN:HD22 | 1:175:A:LEU:H | 13 | 0.62 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 20 | 0.62 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 13 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 1 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 1 | 0.62 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 1 | 0.62 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 14 | 0.62 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 14 | 0.62 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 5 | 0.62 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 7 | 0.62 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 20 | 0.62 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 11 | 0.61 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 11 | 0.61 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 11 | 0.61 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 9 | 0.61 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 9 | 0.61 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 9 | 0.61 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 9 | 0.61 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 9 | 0.61 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 9 | 0.61 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE21 | 14 | 0.61 |
| (1,2003) | 1:58:A:GLN:H | 1:58:A:GLN:HE22 | 14 | 0.61 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 6 | 0.61 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 6 | 0.61 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 6 | 0.61 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 6 | 0.61 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 6 | 0.61 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 6 | 0.61 |
| (1,1885) | 1:25:A:GLN:HE21 | 1:26:A:TRP:H | 9 | 0.61 |
| (1,1885) | 1:25:A:GLN:HE22 | 1:26:A:TRP:H | 9 | 0.61 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 8 | 0.61 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 8 | 0.61 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 12 | 0.61 |
| (1,1483) | 1:34:A:LEU:HD11 | 1:201:A:CYS:HB2 | 9 | 0.61 |
| (1,1483) | 1:34:A:LEU:HD12 | 1:201:A:CYS:HB2 | 9 | 0.61 |
| (1,1483) | 1:34:A:LEU:HD13 | 1:201:A:CYS:HB2 | 9 | 0.61 |
| (1,1483) | 1:34:A:LEU:HD21 | 1:201:A:CYS:HB2 | 9 | 0.61 |
| (1,1483) | 1:34:A:LEU:HD22 | 1:201:A:CYS:HB2 | 9 | 0.61 |
| (1,1483) | 1:34:A:LEU:HD23 | 1:201:A:CYS:HB2 | 9 | 0.61 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 1 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 1 | 0.61 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 1 | 0.61 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 9 | 0.61 |
| (1,1237) | 1:55:A:LEU:HG | 1:56:A:THR:HA | 9 | 0.61 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 8 | 0.61 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 8 | 0.61 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 5 | 0.61 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 17 | 0.61 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 17 | 0.61 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 17 | 0.61 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 18 | 0.61 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 18 | 0.61 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 18 | 0.61 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 3 | 0.61 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 3 | 0.61 |
| (1,2192) | 1:129:A:ARG:HG2 | 1:132:A:CYS:HB2 | 12 | 0.6 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 9 | 0.6 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 13 | 0.6 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 15 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 20 | 0.6 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 20 | 0.6 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 4 | 0.6 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 4 | 0.6 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 4 | 0.6 |
| (1,723) | 1:76:A:SER:H | 1:79:A:VAL:HG11 | 4 | 0.6 |
| (1,723) | 1:76:A:SER:H | 1:79:A:VAL:HG12 | 4 | 0.6 |
| (1,723) | 1:76:A:SER:H | 1:79:A:VAL:HG13 | 4 | 0.6 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 15 | 0.6 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 19 | 0.6 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 19 | 0.6 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 19 | 0.6 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 9 | 0.6 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 2 | 0.6 |
| (1,2) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 8 | 0.6 |
| (1,2) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 8 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD11 | 20 | 0.59 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD12 | 20 | 0.59 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD13 | 20 | 0.59 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD21 | 20 | 0.59 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD22 | 20 | 0.59 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD23 | 20 | 0.59 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 4 | 0.59 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 4 | 0.59 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 4 | 0.59 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 4 | 0.59 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 4 | 0.59 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 4 | 0.59 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 17 | 0.59 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 17 | 0.59 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 17 | 0.59 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 19 | 0.59 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 19 | 0.59 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 19 | 0.59 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 4 | 0.59 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 4 | 0.59 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 4 | 0.59 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 4 | 0.59 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 4 | 0.59 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 4 | 0.59 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 1 | 0.59 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 1 | 0.59 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 5 | 0.59 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 7 | 0.59 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE1 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE2 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE3 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE1 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE2 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE3 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE1 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE2 | 9 | 0.59 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE3 | 9 | 0.59 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 15 | 0.59 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 8 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 20 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 20 | 0.59 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 20 | 0.59 |
| (1,968) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 8 | 0.59 |
| (1,968) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 8 | 0.59 |
| (1,968) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 8 | 0.59 |
| (1,820) | 1:96:A:ILE:HA | 1:99:A:VAL:HB | 17 | 0.59 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 7 | 0.59 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 7 | 0.59 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 7 | 0.59 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 3 | 0.59 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 3 | 0.59 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 3 | 0.59 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 3 | 0.59 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 4 | 0.58 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 4 | 0.58 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 4 | 0.58 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 9 | 0.58 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 9 | 0.58 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 9 | 0.58 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 9 | 0.58 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 10 | 0.58 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 10 | 0.58 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 10 | 0.58 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 13 | 0.58 |
| (1,1863) | 1:13:A:LEU:HD11 | 1:217:A:VAL:HB | 4 | 0.58 |
| (1,1863) | 1:13:A:LEU:HD12 | 1:217:A:VAL:HB | 4 | 0.58 |
| (1,1863) | 1:13:A:LEU:HD13 | 1:217:A:VAL:HB | 4 | 0.58 |
| (1,1863) | 1:13:A:LEU:HD21 | 1:217:A:VAL:HB | 4 | 0.58 |
| (1,1863) | 1:13:A:LEU:HD22 | 1:217:A:VAL:HB | 4 | 0.58 |
| (1,1863) | 1:13:A:LEU:HD23 | 1:217:A:VAL:HB | 4 | 0.58 |
| (1,1830) | 1:7:A:GLU:HG2 | 1:8:A:ILE:HB | 10 | 0.58 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 20 | 0.58 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 20 | 0.58 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 20 | 0.58 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 20 | 0.58 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 1 | 0.58 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 1 | 0.58 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 1 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 1 | 0.58 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 1 | 0.58 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 1 | 0.58 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 3 | 0.58 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 6 | 0.58 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 9 | 0.58 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 3 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 2 | 0.58 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 2 | 0.58 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 2 | 0.58 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 2 | 0.58 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 5 | 0.58 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 5 | 0.58 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 5 | 0.58 |
| (1,1003) | 1:131:A:LYS:HA | 1:134:A:GLU:HB2 | 19 | 0.58 |
| (1,962) | 1:124:A:MET:HE1 | 1:129:A:ARG:H | 8 | 0.58 |
| (1,962) | 1:124:A:MET:HE2 | 1:129:A:ARG:H | 8 | 0.58 |
| (1,962) | 1:124:A:MET:HE3 | 1:129:A:ARG:H | 8 | 0.58 |
| (1,879) | 1:8:A:ILE:HG21 | 1:216:A:ALA:H | 16 | 0.58 |
| (1,879) | 1:8:A:ILE:HG22 | 1:216:A:ALA:H | 16 | 0.58 |
| (1,879) | 1:8:A:ILE:HG23 | 1:216:A:ALA:H | 16 | 0.58 |
| (1,590) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 16 | 0.58 |
| (1,305) | 1:31:A:VAL:H | 1:217:A:VAL:H | 16 | 0.58 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 16 | 0.57 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 16 | 0.57 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 16 | 0.57 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 16 | 0.57 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 16 | 0.57 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 16 | 0.57 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 5 | 0.57 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 5 | 0.57 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 2 | 0.57 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 17 | 0.57 |
| (1,1576) | 1:175:A:LEU:HG | 1:183:A:VAL:H | 3 | 0.57 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB1 | 1 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB2 | 1 | 0.57 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB3 | 1 | 0.57 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 10 | 0.57 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 9 | 0.57 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD21 | 9 | 0.57 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD22 | 9 | 0.57 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD23 | 9 | 0.57 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 18 | 0.57 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 18 | 0.57 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 18 | 0.57 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 2 | 0.57 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 2 | 0.57 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 2 | 0.57 |
| (1,582) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD21 | 13 | 0.57 |
| (1,582) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD21 | 13 | 0.57 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 4 | 0.57 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 16 | 0.57 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 16 | 0.57 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 18 | 0.57 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 18 | 0.57 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 18 | 0.57 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 18 | 0.57 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 18 | 0.57 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 18 | 0.57 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 11 | 0.56 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 11 | 0.56 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 11 | 0.56 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 11 | 0.56 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 11 | 0.56 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 11 | 0.56 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 9 | 0.56 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 20 | 0.56 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 20 | 0.56 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 20 | 0.56 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 20 | 0.56 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 20 | 0.56 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 20 | 0.56 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 2 | 0.56 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 2 | 0.56 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 7 | 0.56 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 7 | 0.56 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 11 | 0.56 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 11 | 0.56 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 11 | 0.56 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 11 | 0.56 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 11 | 0.56 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 11 | 0.56 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 18 | 0.56 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 13 | 0.56 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 13 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 16 | 0.56 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 16 | 0.56 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 6 | 0.56 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 6 | 0.56 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 1 | 0.56 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 12 | 0.56 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 12 | 0.56 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 12 | 0.56 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 11 | 0.56 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD11 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD12 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD13 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD11 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD12 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD13 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD11 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD12 | 5 | 0.56 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD13 | 5 | 0.56 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 3 | 0.56 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 9 | 0.56 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 7 | 0.56 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 15 | 0.56 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 15 | 0.56 |
| (1,496) | 1:53:A:PHE:HB2 | 1:215:A:SER:H | 10 | 0.56 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 6 | 0.56 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 14 | 0.56 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 17 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 20 | 0.56 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 20 | 0.55 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 20 | 0.55 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 17 | 0.55 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 18 | 0.55 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 18 | 0.55 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 18 | 0.55 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 18 | 0.55 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 18 | 0.55 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 18 | 0.55 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 13 | 0.55 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 13 | 0.55 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 13 | 0.55 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 16 | 0.55 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 16 | 0.55 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 9 | 0.55 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 9 | 0.55 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 17 | 0.55 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 1 | 0.55 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 1 | 0.55 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 1 | 0.55 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 5 | 0.55 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 5 | 0.55 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 5 | 0.55 |
| (1,1121) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HG2 | 5 | 0.55 |
| (1,1121) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HG2 | 5 | 0.55 |
| (1,1121) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HG2 | 5 | 0.55 |
| (1,1085) | 1:81:A:PHE:HE1 | 1:175:A:LEU:HB2 | 1 | 0.55 |
| (1,1085) | 1:81:A:PHE:HE2 | 1:175:A:LEU:HB2 | 1 | 0.55 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 17 | 0.55 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 17 | 0.55 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 17 | 0.55 |
| (1,1003) | 1:131:A:LYS:HA | 1:134:A:GLU:HB2 | 16 | 0.55 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG21 | 4 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG22 | 4 | 0.55 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG23 | 4 | 0.55 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 5 | 0.55 |
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 5 | 0.55 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 5 | 0.55 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 8 | 0.55 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 8 | 0.55 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 8 | 0.55 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 17 | 0.55 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 17 | 0.55 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 17 | 0.55 |
| (1,706) | 1:73:A:GLN:HA | 1:74:A:GLU:H | 20 | 0.55 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 9 | 0.55 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 15 | 0.55 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 12 | 0.54 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 12 | 0.54 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 17 | 0.54 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 17 | 0.54 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 17 | 0.54 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 17 | 0.54 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 17 | 0.54 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 17 | 0.54 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 17 | 0.54 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 17 | 0.54 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 13 | 0.54 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 13 | 0.54 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 13 | 0.54 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 13 | 0.54 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 13 | 0.54 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 13 | 0.54 |
| (1,1876) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE21 | 8 | 0.54 |
| (1,1876) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 8 | 0.54 |
| (1,1876) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE21 | 8 | 0.54 |
| (1,1876) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 8 | 0.54 |
| (1,1876) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE21 | 8 | 0.54 |
| (1,1876) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 8 | 0.54 |
| (1,1805) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HB | 11 | 0.54 |
| (1,1805) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HB | 11 | 0.54 |
| (1,1805) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HB | 11 | 0.54 |
| (1,1805) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HB | 11 | 0.54 |
| (1,1805) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HB | 11 | 0.54 |
| (1,1805) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HB | 11 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 12 | 0.54 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 14 | 0.54 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE1 | 18 | 0.54 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE2 | 18 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 11 | 0.54 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 11 | 0.54 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 16 | 0.54 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 6 | 0.54 |
| (1,2285) | 1:167:A:ASN:HD21 | 1:193:A:LEU:HG | 19 | 0.53 |
| (1,2285) | 1:167:A:ASN:HD22 | 1:193:A:LEU:HG | 19 | 0.53 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 5 | 0.53 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 5 | 0.53 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 5 | 0.53 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 5 | 0.53 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 5 | 0.53 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 5 | 0.53 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 5 | 0.53 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 5 | 0.53 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 5 | 0.53 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 5 | 0.53 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 5 | 0.53 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 5 | 0.53 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 8 | 0.53 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 8 | 0.53 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE21 | 17 | 0.53 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE22 | 17 | 0.53 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 4 | 0.53 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 4 | 0.53 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 4 | 0.53 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 3 | 0.53 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 2 | 0.53 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 16 | 0.53 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 16 | 0.53 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 16 | 0.53 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 2 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB1 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB2 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB3 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB1 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB2 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB3 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB1 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB2 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB3 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB1 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB2 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB3 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB1 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB2 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB3 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB1 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB2 | 9 | 0.53 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB3 | 9 | 0.53 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 2 | 0.53 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 16 | 0.53 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 8 | 0.53 |
| (1,1410) | 1:137:A:GLU:H | 1:140:A:GLN:HB2 | 4 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD11 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD12 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD13 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD21 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD22 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD23 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD11 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD12 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD13 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD21 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD22 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD23 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD11 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD12 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD13 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD21 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD22 | 3 | 0.53 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD23 | 3 | 0.53 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 1 | 0.53 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 10 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 10 | 0.53 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 10 | 0.53 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 9 | 0.53 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 1 | 0.53 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 4 | 0.53 |
| (1,586) | 1:67:A:ILE:HD11 | 1:176:A:ASP:H | 18 | 0.53 |
| (1,586) | 1:67:A:ILE:HD12 | 1:176:A:ASP:H | 18 | 0.53 |
| (1,586) | 1:67:A:ILE:HD13 | 1:176:A:ASP:H | 18 | 0.53 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 19 | 0.53 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE1 | 18 | 0.53 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE2 | 18 | 0.53 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE3 | 18 | 0.53 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 4 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 4 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 4 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 4 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 4 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 4 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 8 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 8 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 8 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 8 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 8 | 0.52 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 8 | 0.52 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 13 | 0.52 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 13 | 0.52 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD11 | 7 | 0.52 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD12 | 7 | 0.52 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD13 | 7 | 0.52 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD21 | 7 | 0.52 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD22 | 7 | 0.52 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD23 | 7 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 12 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 12 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 12 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 12 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 12 | 0.52 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 12 | 0.52 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 15 | 0.52 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 15 | 0.52 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 15 | 0.52 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 15 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 15 | 0.52 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 15 | 0.52 |
| (1,1830) | 1:7:A:GLU:HG2 | 1:8:A:ILE:HB | 12 | 0.52 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 14 | 0.52 |
| (1,1673) | 1:115:A:LYS:HE2 | 1:116:A:GLN:HA | 11 | 0.52 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 20 | 0.52 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 13 | 0.52 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 2 | 0.52 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 2 | 0.52 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 18 | 0.52 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 18 | 0.52 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 18 | 0.52 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 10 | 0.52 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 10 | 0.52 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 10 | 0.52 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 17 | 0.52 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 17 | 0.52 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 17 | 0.52 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD11 | 19 | 0.52 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD12 | 19 | 0.52 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD13 | 19 | 0.52 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD11 | 19 | 0.52 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD12 | 19 | 0.52 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD13 | 19 | 0.52 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 11 | 0.52 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 11 | 0.52 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 11 | 0.52 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 11 | 0.52 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 11 | 0.52 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 11 | 0.52 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 8 | 0.52 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 7 | 0.52 |
| (1,674) | 1:223:A:ALA:HA | 1:224:A:LEU:H | 13 | 0.52 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 20 | 0.52 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 12 | 0.52 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 20 | 0.52 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 20 | 0.52 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 16 | 0.52 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 11 | 0.52 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 20 | 0.52 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 11 | 0.52 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 11 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 11 | 0.52 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 11 | 0.52 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 11 | 0.52 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 11 | 0.52 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 2 | 0.51 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 2 | 0.51 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 2 | 0.51 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 2 | 0.51 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 2 | 0.51 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 2 | 0.51 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 11 | 0.51 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 11 | 0.51 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 11 | 0.51 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 11 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 18 | 0.51 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 18 | 0.51 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 3 | 0.51 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 3 | 0.51 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 3 | 0.51 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 3 | 0.51 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 3 | 0.51 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 3 | 0.51 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 16 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 19 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 19 | 0.51 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 19 | 0.51 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 18 | 0.51 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 6 | 0.51 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 16 | 0.51 |
| (1,1224) | 1:163:A:ILE:HD11 | 1:165:A:PHE:H | 3 | 0.51 |
| (1,1224) | 1:163:A:ILE:HD12 | 1:165:A:PHE:H | 3 | 0.51 |
| (1,1224) | 1:163:A:ILE:HD13 | 1:165:A:PHE:H | 3 | 0.51 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 19 | 0.51 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 19 | 0.51 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 19 | 0.51 |
| (1,1003) | 1:131:A:LYS:HA | 1:134:A:GLU:HB2 | 11 | 0.51 |
| (1,964) | 1:124:A:MET:HE1 | 1:132:A:CYS:H | 6 | 0.51 |
| (1,964) | 1:124:A:MET:HE2 | 1:132:A:CYS:H | 6 | 0.51 |
| (1,964) | 1:124:A:MET:HE3 | 1:132:A:CYS:H | 6 | 0.51 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 19 | 0.51 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 19 | 0.51 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 11 | 0.51 |
| (1,254) | 1:209:A:GLN:HG2 | 1:210:A:GLY:H | 12 | 0.51 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG11 | 4 | 0.5 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG12 | 4 | 0.5 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG13 | 4 | 0.5 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG21 | 4 | 0.5 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG22 | 4 | 0.5 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG23 | 4 | 0.5 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 7 | 0.5 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 7 | 0.5 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 7 | 0.5 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 14 | 0.5 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 14 | 0.5 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 14 | 0.5 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 14 | 0.5 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 14 | 0.5 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 14 | 0.5 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 10 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 10 | 0.5 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 11 | 0.5 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 11 | 0.5 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 7 | 0.5 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 6 | 0.5 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 6 | 0.5 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 6 | 0.5 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 6 | 0.5 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 6 | 0.5 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 6 | 0.5 |
| (1,1848) | 1:13:A:LEU:HA | 1:17:A:LEU:HB2 | 11 | 0.5 |
| (1,1710) | 1:37:A:GLU:HG2 | 1:38:A:SER:H | 7 | 0.5 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 9 | 0.5 |
| (1,1575) | 1:175:A:LEU:HG | 1:176:A:ASP:H | 18 | 0.5 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 4 | 0.5 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 4 | 0.5 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 4 | 0.5 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 10 | 0.5 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 10 | 0.5 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 10 | 0.5 |
| (1,1051) | 1:23:A:ALA:HB1 | 1:107:A:GLY:H | 11 | 0.5 |
| (1,1051) | 1:23:A:ALA:HB2 | 1:107:A:GLY:H | 11 | 0.5 |
| (1,1051) | 1:23:A:ALA:HB3 | 1:107:A:GLY:H | 11 | 0.5 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 10 | 0.5 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 10 | 0.5 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 10 | 0.5 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB1 | 1 | 0.5 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB2 | 1 | 0.5 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB3 | 1 | 0.5 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 2 | 0.5 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 2 | 0.5 |
| (1,669) | 1:189:A:SER:H | 1:193:A:LEU:H | 1 | 0.5 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 20 | 0.5 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 18 | 0.5 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 4 | 0.5 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 4 | 0.5 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 4 | 0.5 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 7 | 0.5 |
| (1,350) | 1:208:A:GLU:HG2 | 1:209:A:GLN:H | 16 | 0.5 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG21 | 19 | 0.5 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG22 | 19 | 0.5 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG23 | 19 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 15 | 0.49 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 15 | 0.49 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 15 | 0.49 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 15 | 0.49 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 15 | 0.49 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 15 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 6 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 6 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 9 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 9 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 15 | 0.49 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 15 | 0.49 |
| (1,1885) | 1:25:A:GLN:HE21 | 1:26:A:TRP:H | 8 | 0.49 |
| (1,1885) | 1:25:A:GLN:HE22 | 1:26:A:TRP:H | 8 | 0.49 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 10 | 0.49 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 15 | 0.49 |
| (1,1692) | 1:127:A:GLU:HG2 | 1:128:A:ASP:HB2 | 19 | 0.49 |
| (1,1641) | 1:70:A:LEU:HG | 1:72:A:GLY:H | 5 | 0.49 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 17 | 0.49 |
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 17 | 0.49 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 17 | 0.49 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 17 | 0.49 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 17 | 0.49 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 17 | 0.49 |
| (1,1382) | 1:70:A:LEU:HG | 1:72:A:GLY:HA2 | 11 | 0.49 |
| (1,1295) | 1:3:A:LEU:HG | 1:4:A:LYS:H | 9 | 0.49 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 13 | 0.49 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 12 | 0.49 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD1 | 20 | 0.49 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD2 | 20 | 0.49 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 15 | 0.49 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 15 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 17 | 0.49 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 17 | 0.49 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 17 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD11 | 15 | 0.49 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD12 | 15 | 0.49 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD13 | 15 | 0.49 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD21 | 15 | 0.49 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD22 | 15 | 0.49 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD23 | 15 | 0.49 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB1 | 7 | 0.49 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB2 | 7 | 0.49 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB3 | 7 | 0.49 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 17 | 0.49 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 17 | 0.49 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 17 | 0.49 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 12 | 0.49 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 12 | 0.49 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 12 | 0.49 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 5 | 0.49 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 9 | 0.49 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE1 | 12 | 0.49 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE2 | 12 | 0.49 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE3 | 12 | 0.49 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE21 | 9 | 0.48 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE22 | 9 | 0.48 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 2 | 0.48 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 2 | 0.48 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 2 | 0.48 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 2 | 0.48 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 2 | 0.48 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 2 | 0.48 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 3 | 0.48 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 3 | 0.48 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 3 | 0.48 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 3 | 0.48 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 3 | 0.48 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 3 | 0.48 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 16 | 0.48 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 16 | 0.48 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 2 | 0.48 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 2 | 0.48 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 2 | 0.48 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 2 | 0.48 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 2 | 0.48 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 2 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 1 | 0.48 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 11 | 0.48 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB1 | 2 | 0.48 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB2 | 2 | 0.48 |
| (1,1591) | 1:80:A:TYR:HE1 | 1:100:A:ALA:HB3 | 2 | 0.48 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 11 | 0.48 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 3 | 0.48 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 3 | 0.48 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 3 | 0.48 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 19 | 0.48 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 19 | 0.48 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 19 | 0.48 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 19 | 0.48 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 16 | 0.48 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 13 | 0.48 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 15 | 0.48 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 15 | 0.48 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 15 | 0.48 |
| (1,1011) | 1:19:A:ARG:HD2 | 1:146:A:VAL:HA | 5 | 0.48 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD21 | 6 | 0.48 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD22 | 6 | 0.48 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD23 | 6 | 0.48 |
| (1,574) | 1:164:A:LEU:HG | 1:175:A:LEU:H | 5 | 0.48 |
| (1,301) | 1:8:A:ILE:HG21 | 1:91:A:GLY:H | 20 | 0.48 |
| (1,301) | 1:8:A:ILE:HG22 | 1:91:A:GLY:H | 20 | 0.48 |
| (1,301) | 1:8:A:ILE:HG23 | 1:91:A:GLY:H | 20 | 0.48 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 5 | 0.48 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 15 | 0.48 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 15 | 0.48 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 15 | 0.48 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 15 | 0.48 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 15 | 0.48 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 15 | 0.48 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 18 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 18 | 0.47 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 11 | 0.47 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 11 | 0.47 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 11 | 0.47 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 11 | 0.47 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 11 | 0.47 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 11 | 0.47 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 11 | 0.47 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 11 | 0.47 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 11 | 0.47 |
| (1,1874) | 1:17:A:LEU:HD11 | 1:95:A:LEU:HB2 | 8 | 0.47 |
| (1,1874) | 1:17:A:LEU:HD12 | 1:95:A:LEU:HB2 | 8 | 0.47 |
| (1,1874) | 1:17:A:LEU:HD13 | 1:95:A:LEU:HB2 | 8 | 0.47 |
| (1,1874) | 1:17:A:LEU:HD21 | 1:95:A:LEU:HB2 | 8 | 0.47 |
| (1,1874) | 1:17:A:LEU:HD22 | 1:95:A:LEU:HB2 | 8 | 0.47 |
| (1,1874) | 1:17:A:LEU:HD23 | 1:95:A:LEU:HB2 | 8 | 0.47 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 10 | 0.47 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 10 | 0.47 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 10 | 0.47 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 4 | 0.47 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 18 | 0.47 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 10 | 0.47 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 17 | 0.47 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 17 | 0.47 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 17 | 0.47 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 13 | 0.47 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 20 | 0.47 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 19 | 0.47 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 1 | 0.47 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 1 | 0.47 |
| (1,1121) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HG2 | 8 | 0.47 |
| (1,1121) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HG2 | 8 | 0.47 |
| (1,1121) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HG2 | 8 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 1 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 1 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 1 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 11 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 11 | 0.47 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 11 | 0.47 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 10 | 0.47 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 10 | 0.47 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 10 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,976) | 1:82:A:MET:HE1 | 1:93:A:ILE:H | 5 | 0.47 |
| (1,976) | 1:82:A:MET:HE2 | 1:93:A:ILE:H | 5 | 0.47 |
| (1,976) | 1:82:A:MET:HE3 | 1:93:A:ILE:H | 5 | 0.47 |
| (1,971) | 1:12:A:MET:HE1 | 1:150:A:GLY:H | 8 | 0.47 |
| (1,971) | 1:12:A:MET:HE2 | 1:150:A:GLY:H | 8 | 0.47 |
| (1,971) | 1:12:A:MET:HE3 | 1:150:A:GLY:H | 8 | 0.47 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 5 | 0.47 |
| (1,565) | 1:212:A:VAL:H | 1:213:A:ARG:H | 8 | 0.47 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 9 | 0.47 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 9 | 0.47 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 9 | 0.47 |
| (1,403) | 1:99:A:VAL:HG11 | 1:103:A:GLN:HE21 | 2 | 0.47 |
| (1,403) | 1:99:A:VAL:HG12 | 1:103:A:GLN:HE21 | 2 | 0.47 |
| (1,403) | 1:99:A:VAL:HG13 | 1:103:A:GLN:HE21 | 2 | 0.47 |
| (1,403) | 1:99:A:VAL:HG21 | 1:103:A:GLN:HE21 | 2 | 0.47 |
| (1,403) | 1:99:A:VAL:HG22 | 1:103:A:GLN:HE21 | 2 | 0.47 |
| (1,403) | 1:99:A:VAL:HG23 | 1:103:A:GLN:HE21 | 2 | 0.47 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 3 | 0.47 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 3 | 0.47 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 15 | 0.46 |
| (1,2307) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD21 | 13 | 0.46 |
| (1,2307) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 13 | 0.46 |
| (1,2307) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD21 | 13 | 0.46 |
| (1,2307) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 13 | 0.46 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 17 | 0.46 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 17 | 0.46 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 17 | 0.46 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 17 | 0.46 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 17 | 0.46 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 17 | 0.46 |
| (1,2226) | 1:148:A:GLN:H | 1:148:A:GLN:HG2 | 4 | 0.46 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 14 | 0.46 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 14 | 0.46 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 14 | 0.46 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 14 | 0.46 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 14 | 0.46 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 14 | 0.46 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 4 | 0.46 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 4 | 0.46 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 4 | 0.46 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD11 | 18 | 0.46 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD12 | 18 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD13 | 18 | 0.46 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD21 | 18 | 0.46 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD22 | 18 | 0.46 |
| (1,2071) | 1:80:A:TYR:HE1 | 1:118:A:LEU:HD23 | 18 | 0.46 |
| (1,1997) | 1:55:A:LEU:HD11 | 1:161:A:HIS:H | 18 | 0.46 |
| (1,1997) | 1:55:A:LEU:HD12 | 1:161:A:HIS:H | 18 | 0.46 |
| (1,1997) | 1:55:A:LEU:HD13 | 1:161:A:HIS:H | 18 | 0.46 |
| (1,1997) | 1:55:A:LEU:HD21 | 1:161:A:HIS:H | 18 | 0.46 |
| (1,1997) | 1:55:A:LEU:HD22 | 1:161:A:HIS:H | 18 | 0.46 |
| (1,1997) | 1:55:A:LEU:HD23 | 1:161:A:HIS:H | 18 | 0.46 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 10 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 18 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 18 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 18 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 18 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 18 | 0.46 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 18 | 0.46 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 4 | 0.46 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 4 | 0.46 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 4 | 0.46 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 4 | 0.46 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 4 | 0.46 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 4 | 0.46 |
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 9 | 0.46 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 9 | 0.46 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 4 | 0.46 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 4 | 0.46 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 4 | 0.46 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 4 | 0.46 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 4 | 0.46 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 4 | 0.46 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 18 | 0.46 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 18 | 0.46 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 18 | 0.46 |
| (1,1717) | 1:118:A:LEU:H | 1:120:A:GLU:HG2 | 3 | 0.46 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 12 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 12 | 0.46 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 12 | 0.46 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 12 | 0.46 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 12 | 0.46 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 12 | 0.46 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE1 | 18 | 0.46 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE2 | 18 | 0.46 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE1 | 18 | 0.46 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE2 | 18 | 0.46 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE1 | 18 | 0.46 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE2 | 18 | 0.46 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 18 | 0.46 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 18 | 0.46 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 18 | 0.46 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 3 | 0.46 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 16 | 0.46 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 3 | 0.46 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 8 | 0.46 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 8 | 0.46 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 8 | 0.46 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 12 | 0.46 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 12 | 0.46 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 12 | 0.46 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 11 | 0.46 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 11 | 0.46 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 11 | 0.46 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 1 | 0.46 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 1 | 0.46 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 1 | 0.46 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 16 | 0.46 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 16 | 0.46 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 16 | 0.46 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 3 | 0.46 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 3 | 0.46 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 3 | 0.46 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 3 | 0.46 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 3 | 0.46 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 3 | 0.46 |
| (1,518) | 1:3:A:LEU:H | 1:87:A:GLY:H | 1 | 0.46 |
| (1,458) | 1:156:A:ASP:HA | 1:158:A:VAL:H | 4 | 0.46 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 3 | 0.46 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 3 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 3 | 0.46 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 9 | 0.46 |
| (1,224) | 1:167:A:ASN:HD21 | 1:190:A:GLU:HA | 9 | 0.46 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 7 | 0.46 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 7 | 0.46 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 6 | 0.45 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 10 | 0.45 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 10 | 0.45 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 10 | 0.45 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 10 | 0.45 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 10 | 0.45 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 10 | 0.45 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 7 | 0.45 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 7 | 0.45 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 7 | 0.45 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 7 | 0.45 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 7 | 0.45 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 7 | 0.45 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 17 | 0.45 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 17 | 0.45 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 17 | 0.45 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 17 | 0.45 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 8 | 0.45 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 20 | 0.45 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 5 | 0.45 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 14 | 0.45 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 14 | 0.45 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 14 | 0.45 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 14 | 0.45 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 14 | 0.45 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 14 | 0.45 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 8 | 0.45 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 15 | 0.45 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 8 | 0.45 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 14 | 0.45 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 12 | 0.45 |
| (1,219) | 1:222:A:ALA:HA | 1:223:A:ALA:H | 3 | 0.45 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG11 | 3 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG12 | 3 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG13 | 3 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG21 | 3 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG22 | 3 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG23 | 3 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG11 | 18 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG12 | 18 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG13 | 18 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG21 | 18 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG22 | 18 | 0.44 |
| (1,2263) | 1:166:A:ASN:HB2 | 1:168:A:VAL:HG23 | 18 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 14 | 0.44 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 14 | 0.44 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 16 | 0.44 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 16 | 0.44 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 16 | 0.44 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 16 | 0.44 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 16 | 0.44 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 16 | 0.44 |
| (1,2039) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 13 | 0.44 |
| (1,2039) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 13 | 0.44 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 12 | 0.44 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 12 | 0.44 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 18 | 0.44 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 18 | 0.44 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 18 | 0.44 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 15 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 10 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 10 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 10 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 10 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 10 | 0.44 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 10 | 0.44 |
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 4 | 0.44 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 4 | 0.44 |
| (1,1848) | 1:13:A:LEU:HA | 1:17:A:LEU:HB2 | 1 | 0.44 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 9 | 0.44 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 9 | 0.44 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 9 | 0.44 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 9 | 0.44 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 9 | 0.44 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 9 | 0.44 |
| (1,1622) | 1:51:A:LEU:HD11 | 1:53:A:PHE:HB2 | 7 | 0.44 |
| (1,1622) | 1:51:A:LEU:HD12 | 1:53:A:PHE:HB2 | 7 | 0.44 |
| (1,1622) | 1:51:A:LEU:HD13 | 1:53:A:PHE:HB2 | 7 | 0.44 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 6 | 0.44 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 6 | 0.44 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 6 | 0.44 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 10 | 0.44 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 10 | 0.44 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 10 | 0.44 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 17 | 0.44 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD11 | 16 | 0.44 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD12 | 16 | 0.44 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD13 | 16 | 0.44 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD11 | 19 | 0.44 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD12 | 19 | 0.44 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD13 | 19 | 0.44 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 9 | 0.44 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 9 | 0.44 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 9 | 0.44 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 13 | 0.44 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 13 | 0.44 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 13 | 0.44 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 10 | 0.44 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 10 | 0.44 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 10 | 0.44 |
| (1,1085) | 1:81:A:PHE:HE1 | 1:175:A:LEU:HB2 | 7 | 0.44 |
| (1,1085) | 1:81:A:PHE:HE2 | 1:175:A:LEU:HB2 | 7 | 0.44 |
| (1,940) | 1:154:A:VAL:HG11 | 1:155:A:ASP:HA | 19 | 0.44 |
| (1,940) | 1:154:A:VAL:HG12 | 1:155:A:ASP:HA | 19 | 0.44 |
| (1,940) | 1:154:A:VAL:HG13 | 1:155:A:ASP:HA | 19 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,940) | 1:154:A:VAL:HG21 | 1:155:A:ASP:HA | 19 | 0.44 |
| (1,940) | 1:154:A:VAL:HG22 | 1:155:A:ASP:HA | 19 | 0.44 |
| (1,940) | 1:154:A:VAL:HG23 | 1:155:A:ASP:HA | 19 | 0.44 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 6 | 0.44 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 6 | 0.44 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 6 | 0.44 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 6 | 0.44 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 6 | 0.44 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 6 | 0.44 |
| (1,894) | 1:82:A:MET:HE1 | 1:96:A:ILE:HG21 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE1 | 1:96:A:ILE:HG22 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE1 | 1:96:A:ILE:HG23 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE2 | 1:96:A:ILE:HG21 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE2 | 1:96:A:ILE:HG22 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE2 | 1:96:A:ILE:HG23 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE3 | 1:96:A:ILE:HG21 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE3 | 1:96:A:ILE:HG22 | 13 | 0.44 |
| (1,894) | 1:82:A:MET:HE3 | 1:96:A:ILE:HG23 | 13 | 0.44 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 5 | 0.44 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 18 | 0.44 |
| (1,669) | 1:189:A:SER:H | 1:193:A:LEU:H | 5 | 0.44 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 15 | 0.44 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 15 | 0.44 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 15 | 0.44 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 11 | 0.44 |
| (1,443) | 1:135:A:LYS:H | 1:135:A:LYS:HE2 | 9 | 0.44 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 8 | 0.44 |
| (1,416) | 1:193:A:LEU:HD11 | 1:197:A:ALA:H | 19 | 0.44 |
| (1,416) | 1:193:A:LEU:HD12 | 1:197:A:ALA:H | 19 | 0.44 |
| (1,416) | 1:193:A:LEU:HD13 | 1:197:A:ALA:H | 19 | 0.44 |
| (1,416) | 1:193:A:LEU:HD21 | 1:197:A:ALA:H | 19 | 0.44 |
| (1,416) | 1:193:A:LEU:HD22 | 1:197:A:ALA:H | 19 | 0.44 |
| (1,416) | 1:193:A:LEU:HD23 | 1:197:A:ALA:H | 19 | 0.44 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 6 | 0.44 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 8 | 0.44 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 20 | 0.44 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 20 | 0.44 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 20 | 0.44 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 20 | 0.44 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 20 | 0.44 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 20 | 0.44 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 2 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 2 | 0.43 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 2 | 0.43 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 2 | 0.43 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 2 | 0.43 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 2 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD11 | 5 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD12 | 5 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD13 | 5 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD21 | 5 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD22 | 5 | 0.43 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD23 | 5 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 10 | 0.43 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 10 | 0.43 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 20 | 0.43 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 20 | 0.43 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 19 | 0.43 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 11 | 0.43 |
| (1,1730) | 1:108:A:PHE:HA | 1:109:A:GLU:HG2 | 10 | 0.43 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 6 | 0.43 |
| (1,1663) | 1:23:A:ALA:HA | 1:108:A:PHE:HB2 | 12 | 0.43 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 1 | 0.43 |
| (1,1575) | 1:175:A:LEU:HG | 1:176:A:ASP:H | 3 | 0.43 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 4 | 0.43 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 4 | 0.43 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 4 | 0.43 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 4 | 0.43 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 4 | 0.43 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 16 | 0.43 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 16 | 0.43 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 16 | 0.43 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 2 | 0.43 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 11 | 0.43 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 15 | 0.43 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 5 | 0.43 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 7 | 0.43 |
| (1,1306) | 1:48:A:ALA:HB1 | 1:218:A:ALA:HA | 3 | 0.43 |
| (1,1306) | 1:48:A:ALA:HB2 | 1:218:A:ALA:HA | 3 | 0.43 |
| (1,1306) | 1:48:A:ALA:HB3 | 1:218:A:ALA:HA | 3 | 0.43 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 4 | 0.43 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 5 | 0.43 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 5 | 0.43 |
| (1,801) | 1:56:A:THR:HG21 | 1:57:A:ALA:HA | 1 | 0.43 |
| (1,801) | 1:56:A:THR:HG22 | 1:57:A:ALA:HA | 1 | 0.43 |
| (1,801) | 1:56:A:THR:HG23 | 1:57:A:ALA:HA | 1 | 0.43 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 14 | 0.43 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 14 | 0.43 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 14 | 0.43 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 19 | 0.43 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 15 | 0.43 |
| (1,502) | 1:224:A:LEU:HG | 1:225:A:GLU:H | 9 | 0.43 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 19 | 0.43 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 12 | 0.43 |
| (1,238) | 1:169:A:ASP:H | 1:173:A:TYR:HE1 | 1 | 0.43 |
| (1,238) | 1:169:A:ASP:H | 1:173:A:TYR:HE2 | 1 | 0.43 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 4 | 0.43 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 5 | 0.43 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 15 | 0.43 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 14 | 0.42 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 14 | 0.42 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 14 | 0.42 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 9 | 0.42 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 9 | 0.42 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 9 | 0.42 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 9 | 0.42 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 9 | 0.42 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 9 | 0.42 |
| (1,2272) | 1:167:A:ASN:HB2 | 1:188:A:SER:HB2 | 15 | 0.42 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 1 | 0.42 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 1 | 0.42 |
| (1,1997) | 1:55:A:LEU:HD11 | 1:161:A:HIS:H | 3 | 0.42 |
| (1,1997) | 1:55:A:LEU:HD12 | 1:161:A:HIS:H | 3 | 0.42 |
| (1,1997) | 1:55:A:LEU:HD13 | 1:161:A:HIS:H | 3 | 0.42 |
| (1,1997) | 1:55:A:LEU:HD21 | 1:161:A:HIS:H | 3 | 0.42 |
| (1,1997) | 1:55:A:LEU:HD22 | 1:161:A:HIS:H | 3 | 0.42 |
| (1,1997) | 1:55:A:LEU:HD23 | 1:161:A:HIS:H | 3 | 0.42 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 6 | 0.42 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 9 | 0.42 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 18 | 0.42 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 12 | 0.42 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 12 | 0.42 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 12 | 0.42 |
| (1,1587) | 1:121:A:THR:HG21 | 1:129:A:ARG:HD2 | 7 | 0.42 |
| (1,1587) | 1:121:A:THR:HG22 | 1:129:A:ARG:HD2 | 7 | 0.42 |
| (1,1587) | 1:121:A:THR:HG23 | 1:129:A:ARG:HD2 | 7 | 0.42 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 2 | 0.42 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 2 | 0.42 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 2 | 0.42 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 2 | 0.42 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 2 | 0.42 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 2 | 0.42 |
| (1,1382) | 1:70:A:LEU:HG | 1:72:A:GLY:HA2 | 5 | 0.42 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 18 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 18 | 0.42 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 18 | 0.42 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 10 | 0.42 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 10 | 0.42 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 10 | 0.42 |
| (1,1080) | 1:8:A:ILE:HG12 | 1:90:A:CYS:HA | 2 | 0.42 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 4 | 0.42 |
| (1,351) | 1:208:A:GLU:HA | 1:209:A:GLN:H | 18 | 0.42 |
| (1,30) | 1:23:A:ALA:H | 1:109:A:GLU:H | 16 | 0.42 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE21 | 19 | 0.41 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE22 | 19 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 9 | 0.41 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 9 | 0.41 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 6 | 0.41 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 6 | 0.41 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 6 | 0.41 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 4 | 0.41 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 4 | 0.41 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 4 | 0.41 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 4 | 0.41 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 4 | 0.41 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 4 | 0.41 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 12 | 0.41 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 12 | 0.41 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 12 | 0.41 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 2 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 8 | 0.41 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 8 | 0.41 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 8 | 0.41 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 8 | 0.41 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 8 | 0.41 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 8 | 0.41 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 8 | 0.41 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 16 | 0.41 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 16 | 0.41 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 16 | 0.41 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 16 | 0.41 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 16 | 0.41 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 16 | 0.41 |
| (1,1876) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE21 | 15 | 0.41 |
| (1,1876) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 15 | 0.41 |
| (1,1876) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE21 | 15 | 0.41 |
| (1,1876) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 15 | 0.41 |
| (1,1876) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE21 | 15 | 0.41 |
| (1,1876) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 15 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 13 | 0.41 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 13 | 0.41 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE1 | 15 | 0.41 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE2 | 15 | 0.41 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE3 | 15 | 0.41 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD1 | 8 | 0.41 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD2 | 8 | 0.41 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 4 | 0.41 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 8 | 0.41 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 4 | 0.41 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 4 | 0.41 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 4 | 0.41 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1575) | 1:175:A:LEU:HG | 1:176:A:ASP:H | 4 | 0.41 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 2 | 0.41 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE1 | 10 | 0.41 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE2 | 10 | 0.41 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE1 | 10 | 0.41 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE2 | 10 | 0.41 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE1 | 10 | 0.41 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE2 | 10 | 0.41 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 6 | 0.41 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 4 | 0.41 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 3 | 0.41 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 3 | 0.41 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 3 | 0.41 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 20 | 0.41 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 20 | 0.41 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 20 | 0.41 |
| (1,964) | 1:124:A:MET:HE1 | 1:132:A:CYS:H | 8 | 0.41 |
| (1,964) | 1:124:A:MET:HE2 | 1:132:A:CYS:H | 8 | 0.41 |
| (1,964) | 1:124:A:MET:HE3 | 1:132:A:CYS:H | 8 | 0.41 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 1 | 0.41 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 1 | 0.41 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 6 | 0.41 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 6 | 0.41 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 11 | 0.41 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 11 | 0.41 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 6 | 0.41 |
| (1,737) | 1:164:A:LEU:H | 1:177:A:GLY:H | 20 | 0.41 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD1 | 16 | 0.41 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD2 | 16 | 0.41 |
| (1,676) | 1:171:A:HIS:H | 1:171:A:HIS:HD2 | 9 | 0.41 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 8 | 0.41 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 17 | 0.41 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 5 | 0.41 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 12 | 0.41 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 18 | 0.41 |
| (1,52) | 1:32:A:LEU:H | 1:32:A:LEU:HG | 15 | 0.41 |
| (1,2234) | 1:157:A:LYS:H | 1:158:A:VAL:HG11 | 4 | 0.4 |
| (1,2234) | 1:157:A:LYS:H | 1:158:A:VAL:HG12 | 4 | 0.4 |
| (1,2234) | 1:157:A:LYS:H | 1:158:A:VAL:HG13 | 4 | 0.4 |
| (1,2234) | 1:157:A:LYS:H | 1:158:A:VAL:HG21 | 4 | 0.4 |
| (1,2234) | 1:157:A:LYS:H | 1:158:A:VAL:HG22 | 4 | 0.4 |
| (1,2234) | 1:157:A:LYS:H | 1:158:A:VAL:HG23 | 4 | 0.4 |
| (1,2202) | 1:136:A:ASN:H | 1:140:A:GLN:HE21 | 10 | 0.4 |
| (1,2202) | 1:136:A:ASN:H | 1:140:A:GLN:HE22 | 10 | 0.4 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 9 | 0.4 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 9 | 0.4 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 9 | 0.4 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 9 | 0.4 |
| (1,1763) | 1:19:A:ARG:HB2 | 1:20:A:LEU:HA | 16 | 0.4 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 5 | 0.4 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 12 | 0.4 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 12 | 0.4 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 12 | 0.4 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 19 | 0.4 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 19 | 0.4 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 19 | 0.4 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 16 | 0.4 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 16 | 0.4 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 16 | 0.4 |
| (1,1299) | 1:52:A:LEU:HG | 1:160:A:PHE:HD1 | 7 | 0.4 |
| (1,1299) | 1:52:A:LEU:HG | 1:160:A:PHE:HD2 | 7 | 0.4 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 3 | 0.4 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 3 | 0.4 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 4 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 18 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 18 | 0.4 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 18 | 0.4 |
| (1,1081) | 1:27:A:ARG:H | 1:28:A:PHE:HA | 3 | 0.4 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 7 | 0.4 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 4 | 0.4 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 4 | 0.4 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 4 | 0.4 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 4 | 0.4 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 4 | 0.4 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 4 | 0.4 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 14 | 0.4 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 14 | 0.4 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 14 | 0.4 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD11 | 17 | 0.4 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD12 | 17 | 0.4 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD13 | 17 | 0.4 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD21 | 17 | 0.4 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD22 | 17 | 0.4 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD23 | 17 | 0.4 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 14 | 0.4 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 20 | 0.4 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 20 | 0.4 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 9 | 0.4 |
| (1,491) | 1:211:A:GLU:HA | 1:212:A:VAL:H | 4 | 0.4 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 18 | 0.4 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 4 | 0.4 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 4 | 0.4 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 4 | 0.4 |
| (1,163) | 1:151:A:GLN:HB2 | 1:152:A:CYS:H | 14 | 0.4 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 13 | 0.4 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 13 | 0.4 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 13 | 0.4 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 13 | 0.4 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 13 | 0.4 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 13 | 0.4 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 6 | 0.39 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 6 | 0.39 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 6 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 18 | 0.39 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 18 | 0.39 |
| (1,2062) | 1:79:A:VAL:HG11 | 1:168:A:VAL:H | 13 | 0.39 |
| (1,2062) | 1:79:A:VAL:HG12 | 1:168:A:VAL:H | 13 | 0.39 |
| (1,2062) | 1:79:A:VAL:HG13 | 1:168:A:VAL:H | 13 | 0.39 |
| (1,2062) | 1:79:A:VAL:HG21 | 1:168:A:VAL:H | 13 | 0.39 |
| (1,2062) | 1:79:A:VAL:HG22 | 1:168:A:VAL:H | 13 | 0.39 |
| (1,2062) | 1:79:A:VAL:HG23 | 1:168:A:VAL:H | 13 | 0.39 |
| (1,2031) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HA | 10 | 0.39 |
| (1,2031) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HA | 10 | 0.39 |
| (1,2031) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HA | 10 | 0.39 |
| (1,2031) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HA | 10 | 0.39 |
| (1,2031) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HA | 10 | 0.39 |
| (1,2031) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HA | 10 | 0.39 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 19 | 0.39 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 19 | 0.39 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 8 | 0.39 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 20 | 0.39 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 20 | 0.39 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 20 | 0.39 |
| (1,1676) | 1:25:A:GLN:HG2 | 1:221:A:LYS:HE2 | 1 | 0.39 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 12 | 0.39 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 1 | 0.39 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 2 | 0.39 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 16 | 0.39 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 1 | 0.39 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 9 | 0.39 |
| (1,1461) | 1:133:A:PHE:HB2 | 1:135:A:LYS:HG2 | 20 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD21 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD22 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD23 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD21 | 12 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD22 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD23 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD21 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD22 | 12 | 0.39 |
| (1,1460) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD23 | 12 | 0.39 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 1 | 0.39 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 1 | 0.39 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 1 | 0.39 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 10 | 0.39 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 7 | 0.39 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 2 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 16 | 0.39 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 16 | 0.39 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD11 | 15 | 0.39 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD12 | 15 | 0.39 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD13 | 15 | 0.39 |
| (1,1189) | 1:34:A:LEU:H | 1:38:A:SER:HB2 | 8 | 0.39 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 1 | 0.39 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 9 | 0.39 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 16 | 0.39 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 16 | 0.39 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 16 | 0.39 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 8 | 0.39 |
| (1,1045) | 1:67:A:ILE:HA | 1:70:A:LEU:HB2 | 4 | 0.39 |
| (1,974) | 1:82:A:MET:HE1 | 1:92:A:THR:HB | 17 | 0.39 |
| (1,974) | 1:82:A:MET:HE2 | 1:92:A:THR:HB | 17 | 0.39 |
| (1,974) | 1:82:A:MET:HE3 | 1:92:A:THR:HB | 17 | 0.39 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 2 | 0.39 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 3 | 0.39 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD11 | 17 | 0.39 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD12 | 17 | 0.39 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD13 | 17 | 0.39 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 19 | 0.39 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 19 | 0.39 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 19 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,745) | 1:55:A:LEU:H | 1:160:A:PHE:HB2 | 12 | 0.39 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 18 | 0.39 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 4 | 0.39 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 5 | 0.39 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 15 | 0.39 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 15 | 0.39 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 15 | 0.39 |
| (1,60) | 1:36:A:GLU:HB2 | 1:37:A:GLU:H | 9 | 0.39 |
| (1,56) | 1:31:A:VAL:HG11 | 1:33:A:GLY:H | 8 | 0.39 |
| (1,56) | 1:31:A:VAL:HG12 | 1:33:A:GLY:H | 8 | 0.39 |
| (1,56) | 1:31:A:VAL:HG13 | 1:33:A:GLY:H | 8 | 0.39 |
| (1,56) | 1:31:A:VAL:HG21 | 1:33:A:GLY:H | 8 | 0.39 |
| (1,56) | 1:31:A:VAL:HG22 | 1:33:A:GLY:H | 8 | 0.39 |
| (1,56) | 1:31:A:VAL:HG23 | 1:33:A:GLY:H | 8 | 0.39 |
| (1,2320) | 1:183:A:VAL:HG11 | 1:185:A:HIS:HA | 5 | 0.38 |
| (1,2320) | 1:183:A:VAL:HG12 | 1:185:A:HIS:HA | 5 | 0.38 |
| (1,2320) | 1:183:A:VAL:HG13 | 1:185:A:HIS:HA | 5 | 0.38 |
| (1,2320) | 1:183:A:VAL:HG21 | 1:185:A:HIS:HA | 5 | 0.38 |
| (1,2320) | 1:183:A:VAL:HG22 | 1:185:A:HIS:HA | 5 | 0.38 |
| (1,2320) | 1:183:A:VAL:HG23 | 1:185:A:HIS:HA | 5 | 0.38 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 13 | 0.38 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 13 | 0.38 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 13 | 0.38 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 13 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 11 | 0.38 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 11 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE21 | 5 | 0.38 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE22 | 5 | 0.38 |
| (1,2012) | 1:58:A:GLN:HG2 | 1:61:A:ASN:HD21 | 11 | 0.38 |
| (1,2012) | 1:58:A:GLN:HG2 | 1:61:A:ASN:HD22 | 11 | 0.38 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 4 | 0.38 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 10 | 0.38 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 10 | 0.38 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 10 | 0.38 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 10 | 0.38 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 10 | 0.38 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 10 | 0.38 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 10 | 0.38 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 13 | 0.38 |
| (1,1763) | 1:19:A:ARG:HB2 | 1:20:A:LEU:HA | 5 | 0.38 |
| (1,1745) | 1:31:A:VAL:HB | 1:218:A:ALA:H | 12 | 0.38 |
| (1,1676) | 1:25:A:GLN:HG2 | 1:221:A:LYS:HE2 | 2 | 0.38 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 12 | 0.38 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 6 | 0.38 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 19 | 0.38 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 19 | 0.38 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 19 | 0.38 |
| (1,1576) | 1:175:A:LEU:HG | 1:183:A:VAL:H | 18 | 0.38 |
| (1,1488) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HA | 2 | 0.38 |
| (1,1466) | 1:19:A:ARG:HD2 | 1:145:A:ALA:H | 7 | 0.38 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 19 | 0.38 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD21 | 12 | 0.38 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD22 | 12 | 0.38 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD23 | 12 | 0.38 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 18 | 0.38 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 18 | 0.38 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 18 | 0.38 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 3 | 0.38 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 3 | 0.38 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 3 | 0.38 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 8 | 0.38 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 8 | 0.38 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 8 | 0.38 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 6 | 0.38 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 6 | 0.38 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 6 | 0.38 |
| (1,971) | 1:12:A:MET:HE1 | 1:150:A:GLY:H | 5 | 0.38 |
| (1,971) | 1:12:A:MET:HE2 | 1:150:A:GLY:H | 5 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,971) | 1:12:A:MET:HE3 | 1:150:A:GLY:H | 5 | 0.38 |
| (1,933) | 1:11:A:GLU:HA | 1:11:A:GLU:HG2 | 9 | 0.38 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 3 | 0.38 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 3 | 0.38 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 4 | 0.38 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 4 | 0.38 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 4 | 0.38 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 4 | 0.38 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 4 | 0.38 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 4 | 0.38 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 11 | 0.38 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 11 | 0.38 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 11 | 0.38 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 15 | 0.38 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 15 | 0.38 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 15 | 0.38 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 15 | 0.38 |
| (1,706) | 1:73:A:GLN:HA | 1:74:A:GLU:H | 1 | 0.38 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 16 | 0.38 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 9 | 0.38 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 9 | 0.38 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 9 | 0.38 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 7 | 0.38 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 4 | 0.38 |
| (1,361) | 1:15:A:LYS:H | 1:15:A:LYS:HE2 | 14 | 0.38 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE2 | 6 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 6 | 0.38 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 6 | 0.38 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 13 | 0.38 |
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 13 | 0.38 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 13 | 0.38 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 20 | 0.38 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 20 | 0.38 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 20 | 0.38 |
| (1,317) | 1:206:A:GLU:H | 1:208:A:GLU:H | 5 | 0.38 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 12 | 0.38 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 12 | 0.38 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 14 | 0.38 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 14 | 0.38 |
| (1,60) | 1:36:A:GLU:HB2 | 1:37:A:GLU:H | 11 | 0.38 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 15 | 0.38 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 15 | 0.38 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 15 | 0.38 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 15 | 0.38 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 15 | 0.38 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 15 | 0.38 |
| (1,2) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 9 | 0.38 |
| (1,2) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 9 | 0.38 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 4 | 0.37 |
| (1,2345) | 1:200:A:VAL:HG11 | 1:203:A:GLU:HG2 | 10 | 0.37 |
| (1,2345) | 1:200:A:VAL:HG12 | 1:203:A:GLU:HG2 | 10 | 0.37 |
| (1,2345) | 1:200:A:VAL:HG13 | 1:203:A:GLU:HG2 | 10 | 0.37 |
| (1,2345) | 1:200:A:VAL:HG21 | 1:203:A:GLU:HG2 | 10 | 0.37 |
| (1,2345) | 1:200:A:VAL:HG22 | 1:203:A:GLU:HG2 | 10 | 0.37 |
| (1,2345) | 1:200:A:VAL:HG23 | 1:203:A:GLU:HG2 | 10 | 0.37 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 16 | 0.37 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 16 | 0.37 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 16 | 0.37 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 16 | 0.37 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 16 | 0.37 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 16 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB1 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB2 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB3 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB1 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB2 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB3 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB1 | 20 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB2 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB3 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB1 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB2 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB3 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB1 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB2 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB3 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB1 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB2 | 20 | 0.37 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB3 | 20 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 4 | 0.37 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 4 | 0.37 |
| (1,1995) | 1:55:A:LEU:HD11 | 1:160:A:PHE:H | 18 | 0.37 |
| (1,1995) | 1:55:A:LEU:HD12 | 1:160:A:PHE:H | 18 | 0.37 |
| (1,1995) | 1:55:A:LEU:HD13 | 1:160:A:PHE:H | 18 | 0.37 |
| (1,1995) | 1:55:A:LEU:HD21 | 1:160:A:PHE:H | 18 | 0.37 |
| (1,1995) | 1:55:A:LEU:HD22 | 1:160:A:PHE:H | 18 | 0.37 |
| (1,1995) | 1:55:A:LEU:HD23 | 1:160:A:PHE:H | 18 | 0.37 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 17 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD11 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD12 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD13 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD21 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD22 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD23 | 12 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1837) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD11 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD12 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD13 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD21 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD22 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD23 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD11 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD12 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD13 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD21 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD22 | 12 | 0.37 |
| (1,1837) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD23 | 12 | 0.37 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 6 | 0.37 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 1 | 0.37 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 2 | 0.37 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 7 | 0.37 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 18 | 0.37 |
| (1,1676) | 1:25:A:GLN:HG2 | 1:221:A:LYS:HE2 | 5 | 0.37 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 17 | 0.37 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 15 | 0.37 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 1 | 0.37 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 1 | 0.37 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 1 | 0.37 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 10 | 0.37 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 17 | 0.37 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 20 | 0.37 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 20 | 0.37 |
| (1,1187) | 1:32:A:LEU:H | 1:38:A:SER:HB2 | 10 | 0.37 |
| (1,1185) | 1:172:A:LEU:HA | 1:188:A:SER:HB2 | 15 | 0.37 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 9 | 0.37 |
| (1,1155) | 1:22:A:VAL:HA | 1:108:A:PHE:HA | 16 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 5 | 0.37 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 5 | 0.37 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 8 | 0.37 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 9 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 9 | 0.37 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 9 | 0.37 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 9 | 0.37 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 9 | 0.37 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 9 | 0.37 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 20 | 0.37 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 20 | 0.37 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 5 | 0.37 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 19 | 0.37 |
| (1,879) | 1:8:A:ILE:HG21 | 1:216:A:ALA:H | 4 | 0.37 |
| (1,879) | 1:8:A:ILE:HG22 | 1:216:A:ALA:H | 4 | 0.37 |
| (1,879) | 1:8:A:ILE:HG23 | 1:216:A:ALA:H | 4 | 0.37 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 4 | 0.37 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 11 | 0.37 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 1 | 0.37 |
| (1,427) | 1:212:A:VAL:HG11 | 1:214:A:PHE:H | 12 | 0.37 |
| (1,427) | 1:212:A:VAL:HG12 | 1:214:A:PHE:H | 12 | 0.37 |
| (1,427) | 1:212:A:VAL:HG13 | 1:214:A:PHE:H | 12 | 0.37 |
| (1,427) | 1:212:A:VAL:HG21 | 1:214:A:PHE:H | 12 | 0.37 |
| (1,427) | 1:212:A:VAL:HG22 | 1:214:A:PHE:H | 12 | 0.37 |
| (1,427) | 1:212:A:VAL:HG23 | 1:214:A:PHE:H | 12 | 0.37 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 18 | 0.37 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 1 | 0.36 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 1 | 0.36 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 1 | 0.36 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 10 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 10 | 0.36 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 10 | 0.36 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 10 | 0.36 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 10 | 0.36 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 10 | 0.36 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 19 | 0.36 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 19 | 0.36 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 17 | 0.36 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 17 | 0.36 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 17 | 0.36 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 17 | 0.36 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 17 | 0.36 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 17 | 0.36 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 19 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD11 | 1:53:A:PHE:HD1 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD11 | 1:53:A:PHE:HD2 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD12 | 1:53:A:PHE:HD1 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD12 | 1:53:A:PHE:HD2 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD13 | 1:53:A:PHE:HD1 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD13 | 1:53:A:PHE:HD2 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD21 | 1:53:A:PHE:HD1 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD21 | 1:53:A:PHE:HD2 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD22 | 1:53:A:PHE:HD1 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD22 | 1:53:A:PHE:HD2 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD23 | 1:53:A:PHE:HD1 | 15 | 0.36 |
| (1,1972) | 1:51:A:LEU:HD23 | 1:53:A:PHE:HD2 | 15 | 0.36 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 2 | 0.36 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 2 | 0.36 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 2 | 0.36 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 2 | 0.36 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 2 | 0.36 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 2 | 0.36 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 4 | 0.36 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 4 | 0.36 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 6 | 0.36 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 6 | 0.36 |
| (1,1730) | 1:108:A:PHE:HA | 1:109:A:GLU:HG2 | 4 | 0.36 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 20 | 0.36 |
| (1,1681) | 1:196:A:ASP:HB2 | 1:199:A:LYS:HB2 | 20 | 0.36 |
| (1,1673) | 1:115:A:LYS:HE2 | 1:116:A:GLN:HA | 8 | 0.36 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 20 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG11 | 8 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG12 | 8 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG13 | 8 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG21 | 8 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG22 | 8 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG23 | 8 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG11 | 16 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG12 | 16 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG13 | 16 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG21 | 16 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG22 | 16 | 0.36 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG23 | 16 | 0.36 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 7 | 0.36 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 19 | 0.36 |
| (1,1433) | 1:154:A:VAL:HG11 | 1:156:A:ASP:HA | 6 | 0.36 |
| (1,1433) | 1:154:A:VAL:HG12 | 1:156:A:ASP:HA | 6 | 0.36 |
| (1,1433) | 1:154:A:VAL:HG13 | 1:156:A:ASP:HA | 6 | 0.36 |
| (1,1433) | 1:154:A:VAL:HG21 | 1:156:A:ASP:HA | 6 | 0.36 |
| (1,1433) | 1:154:A:VAL:HG22 | 1:156:A:ASP:HA | 6 | 0.36 |
| (1,1433) | 1:154:A:VAL:HG23 | 1:156:A:ASP:HA | 6 | 0.36 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 20 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 15 | 0.36 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 15 | 0.36 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 9 | 0.36 |
| (1,1237) | 1:55:A:LEU:HG | 1:56:A:THR:HA | 16 | 0.36 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD11 | 14 | 0.36 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD12 | 14 | 0.36 |
| (1,1227) | 1:51:A:LEU:HA | 1:163:A:ILE:HD13 | 14 | 0.36 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 11 | 0.36 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 19 | 0.36 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 10 | 0.36 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 10 | 0.36 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 18 | 0.36 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 18 | 0.36 |
| (1,1189) | 1:34:A:LEU:H | 1:38:A:SER:HB2 | 15 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 3 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 3 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 3 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 14 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 14 | 0.36 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 14 | 0.36 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 16 | 0.36 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 16 | 0.36 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 16 | 0.36 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 11 | 0.36 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 11 | 0.36 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 11 | 0.36 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 4 | 0.36 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 15 | 0.36 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 19 | 0.36 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 19 | 0.36 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 19 | 0.36 |
| (1,976) | 1:82:A:MET:HE1 | 1:93:A:ILE:H | 8 | 0.36 |
| (1,976) | 1:82:A:MET:HE2 | 1:93:A:ILE:H | 8 | 0.36 |
| (1,976) | 1:82:A:MET:HE3 | 1:93:A:ILE:H | 8 | 0.36 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE1 | 7 | 0.36 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE2 | 7 | 0.36 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE3 | 7 | 0.36 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE1 | 12 | 0.36 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE2 | 12 | 0.36 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE3 | 12 | 0.36 |
| (1,933) | 1:11:A:GLU:HA | 1:11:A:GLU:HG2 | 2 | 0.36 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 16 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 16 | 0.36 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 16 | 0.36 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 13 | 0.36 |
| (1,879) | 1:8:A:ILE:HG21 | 1:216:A:ALA:H | 7 | 0.36 |
| (1,879) | 1:8:A:ILE:HG22 | 1:216:A:ALA:H | 7 | 0.36 |
| (1,879) | 1:8:A:ILE:HG23 | 1:216:A:ALA:H | 7 | 0.36 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 9 | 0.36 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG21 | 2 | 0.36 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG22 | 2 | 0.36 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG23 | 2 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD11 | 12 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD12 | 12 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD13 | 12 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD21 | 12 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD22 | 12 | 0.36 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD23 | 12 | 0.36 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 2 | 0.36 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 2 | 0.36 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 2 | 0.36 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 2 | 0.36 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 2 | 0.36 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 2 | 0.36 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 1 | 0.36 |
| (1,351) | 1:208:A:GLU:HA | 1:209:A:GLN:H | 11 | 0.36 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 2 | 0.36 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 1 | 0.36 |
| (1,60) | 1:36:A:GLU:HB2 | 1:37:A:GLU:H | 5 | 0.36 |
| (1,2290) | 1:168:A:VAL:HG11 | 1:169:A:ASP:HA | 19 | 0.35 |
| (1,2290) | 1:168:A:VAL:HG12 | 1:169:A:ASP:HA | 19 | 0.35 |
| (1,2290) | 1:168:A:VAL:HG13 | 1:169:A:ASP:HA | 19 | 0.35 |
| (1,2290) | 1:168:A:VAL:HG21 | 1:169:A:ASP:HA | 19 | 0.35 |
| (1,2290) | 1:168:A:VAL:HG22 | 1:169:A:ASP:HA | 19 | 0.35 |
| (1,2290) | 1:168:A:VAL:HG23 | 1:169:A:ASP:HA | 19 | 0.35 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 3 | 0.35 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 3 | 0.35 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 3 | 0.35 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 3 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 12 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 12 | 0.35 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 12 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 8 | 0.35 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 8 | 0.35 |
| (1,2142) | 1:109:A:GLU:HB2 | 1:110:A:ASP:H | 16 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 11 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 11 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 11 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 11 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 11 | 0.35 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 11 | 0.35 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE21 | 16 | 0.35 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE22 | 16 | 0.35 |
| (1,1997) | 1:55:A:LEU:HD11 | 1:161:A:HIS:H | 9 | 0.35 |
| (1,1997) | 1:55:A:LEU:HD12 | 1:161:A:HIS:H | 9 | 0.35 |
| (1,1997) | 1:55:A:LEU:HD13 | 1:161:A:HIS:H | 9 | 0.35 |
| (1,1997) | 1:55:A:LEU:HD21 | 1:161:A:HIS:H | 9 | 0.35 |
| (1,1997) | 1:55:A:LEU:HD22 | 1:161:A:HIS:H | 9 | 0.35 |
| (1,1997) | 1:55:A:LEU:HD23 | 1:161:A:HIS:H | 9 | 0.35 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 7 | 0.35 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 7 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 7 | 0.35 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 11 | 0.35 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 18 | 0.35 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 18 | 0.35 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 18 | 0.35 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 18 | 0.35 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 18 | 0.35 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 18 | 0.35 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 1 | 0.35 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 1 | 0.35 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 1 | 0.35 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 16 | 0.35 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 16 | 0.35 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 16 | 0.35 |
| (1,1732) | 1:122:A:GLU:HG2 | 1:123:A:LYS:HG2 | 1 | 0.35 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 17 | 0.35 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 2 | 0.35 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 6 | 0.35 |
| (1,1588) | 1:100:A:ALA:HB1 | 1:118:A:LEU:HG | 5 | 0.35 |
| (1,1588) | 1:100:A:ALA:HB2 | 1:118:A:LEU:HG | 5 | 0.35 |
| (1,1588) | 1:100:A:ALA:HB3 | 1:118:A:LEU:HG | 5 | 0.35 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 18 | 0.35 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 18 | 0.35 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 18 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 1 | 0.35 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 1 | 0.35 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD11 | 4 | 0.35 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD12 | 4 | 0.35 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD13 | 4 | 0.35 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD21 | 4 | 0.35 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD22 | 4 | 0.35 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD23 | 4 | 0.35 |
| (1,1261) | 1:70:A:LEU:HA | 1:70:A:LEU:HG | 10 | 0.35 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD1 | 13 | 0.35 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD2 | 13 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1203) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HD1 | 6 | 0.35 |
| (1,1203) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HD2 | 6 | 0.35 |
| (1,1203) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HD1 | 6 | 0.35 |
| (1,1203) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HD2 | 6 | 0.35 |
| (1,1203) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HD1 | 6 | 0.35 |
| (1,1203) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HD2 | 6 | 0.35 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 14 | 0.35 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 14 | 0.35 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 14 | 0.35 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 14 | 0.35 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 14 | 0.35 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 14 | 0.35 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 19 | 0.35 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 19 | 0.35 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 15 | 0.35 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD11 | 17 | 0.35 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD12 | 17 | 0.35 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD13 | 17 | 0.35 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD11 | 17 | 0.35 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD12 | 17 | 0.35 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD13 | 17 | 0.35 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 8 | 0.35 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 16 | 0.35 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 16 | 0.35 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 16 | 0.35 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 13 | 0.35 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD11 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD12 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD13 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD11 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD12 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD13 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD11 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD12 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD13 | 7 | 0.35 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD11 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD12 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD13 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD11 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD12 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD13 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD11 | 17 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD12 | 17 | 0.35 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD13 | 17 | 0.35 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 20 | 0.35 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 20 | 0.35 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 20 | 0.35 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 16 | 0.35 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD1 | 14 | 0.35 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD2 | 14 | 0.35 |
| (1,576) | 1:171:A:HIS:HD2 | 1:172:A:LEU:H | 2 | 0.35 |
| (1,557) | 1:74:A:GLU:HB2 | 1:75:A:VAL:H | 9 | 0.35 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 15 | 0.35 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 15 | 0.35 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 15 | 0.35 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 15 | 0.35 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 15 | 0.35 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 15 | 0.35 |
| (1,465) | 1:168:A:VAL:H | 1:173:A:TYR:HE1 | 1 | 0.35 |
| (1,465) | 1:168:A:VAL:H | 1:173:A:TYR:HE2 | 1 | 0.35 |
| (1,443) | 1:135:A:LYS:H | 1:135:A:LYS:HE2 | 1 | 0.35 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 16 | 0.35 |
| (1,285) | 1:9:A:ASN:HB2 | 1:12:A:MET:H | 7 | 0.35 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 3 | 0.35 |
| (1,60) | 1:36:A:GLU:HB2 | 1:37:A:GLU:H | 17 | 0.35 |
| (1,56) | 1:31:A:VAL:HG11 | 1:33:A:GLY:H | 18 | 0.35 |
| (1,56) | 1:31:A:VAL:HG12 | 1:33:A:GLY:H | 18 | 0.35 |
| (1,56) | 1:31:A:VAL:HG13 | 1:33:A:GLY:H | 18 | 0.35 |
| (1,56) | 1:31:A:VAL:HG21 | 1:33:A:GLY:H | 18 | 0.35 |
| (1,56) | 1:31:A:VAL:HG22 | 1:33:A:GLY:H | 18 | 0.35 |
| (1,56) | 1:31:A:VAL:HG23 | 1:33:A:GLY:H | 18 | 0.35 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 11 | 0.34 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 13 | 0.34 |
| (1,2066) | 1:79:A:VAL:HG11 | 1:173:A:TYR:H | 13 | 0.34 |
| (1,2066) | 1:79:A:VAL:HG12 | 1:173:A:TYR:H | 13 | 0.34 |
| (1,2066) | 1:79:A:VAL:HG13 | 1:173:A:TYR:H | 13 | 0.34 |
| (1,2066) | 1:79:A:VAL:HG21 | 1:173:A:TYR:H | 13 | 0.34 |
| (1,2066) | 1:79:A:VAL:HG22 | 1:173:A:TYR:H | 13 | 0.34 |
| (1,2066) | 1:79:A:VAL:HG23 | 1:173:A:TYR:H | 13 | 0.34 |
| (1,2063) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HB | 13 | 0.34 |
| (1,2063) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HB | 13 | 0.34 |
| (1,2063) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HB | 13 | 0.34 |
| (1,2063) | 1:79:A:VAL:HG21 | 1:168:A:VAL:HB | 13 | 0.34 |
| (1,2063) | 1:79:A:VAL:HG22 | 1:168:A:VAL:HB | 13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2063) | 1:79:A:VAL:HG23 | 1:168:A:VAL:HB | 13 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HD21 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HD22 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HD21 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HD22 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HD21 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HD22 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HD21 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HD22 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HD21 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HD22 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HD21 | 4 | 0.34 |
| (1,2032) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HD22 | 4 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD1 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD2 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD1 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD2 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD1 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD2 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD1 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD2 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD1 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD2 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD1 | 2 | 0.34 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD2 | 2 | 0.34 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 3 | 0.34 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 10 | 0.34 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 17 | 0.34 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 17 | 0.34 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 17 | 0.34 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 17 | 0.34 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 17 | 0.34 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 17 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 8 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 8 | 0.34 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 8 | 0.34 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 9 | 0.34 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 9 | 0.34 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 9 | 0.34 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 9 | 0.34 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 9 | 0.34 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 9 | 0.34 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 4 | 0.34 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 4 | 0.34 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 4 | 0.34 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 19 | 0.34 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 19 | 0.34 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 16 | 0.34 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 19 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 9 | 0.34 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 9 | 0.34 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 19 | 0.34 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 16 | 0.34 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB1 | 2 | 0.34 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB2 | 2 | 0.34 |
| (1,1609) | 1:31:A:VAL:HB | 1:218:A:ALA:HB3 | 2 | 0.34 |
| (1,1575) | 1:175:A:LEU:HG | 1:176:A:ASP:H | 8 | 0.34 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 14 | 0.34 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 6 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 6 | 0.34 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 6 | 0.34 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 1 | 0.34 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 6 | 0.34 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 6 | 0.34 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 6 | 0.34 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG11 | 5 | 0.34 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG12 | 5 | 0.34 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG13 | 5 | 0.34 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG21 | 5 | 0.34 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG22 | 5 | 0.34 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG23 | 5 | 0.34 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 2 | 0.34 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 6 | 0.34 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 6 | 0.34 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 6 | 0.34 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 13 | 0.34 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 13 | 0.34 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 13 | 0.34 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 14 | 0.34 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 14 | 0.34 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 14 | 0.34 |
| (1,1056) | 1:52:A:LEU:HB2 | 1:214:A:PHE:HD1 | 12 | 0.34 |
| (1,1056) | 1:52:A:LEU:HB2 | 1:214:A:PHE:HD2 | 12 | 0.34 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 20 | 0.34 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 16 | 0.34 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 8 | 0.34 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 8 | 0.34 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 8 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 15 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 15 | 0.34 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 15 | 0.34 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD11 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD12 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD13 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD11 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD12 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD13 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD11 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD12 | 5 | 0.34 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD13 | 5 | 0.34 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 18 | 0.34 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 18 | 0.34 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 18 | 0.34 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 18 | 0.34 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 18 | 0.34 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 18 | 0.34 |
| (1,820) | 1:96:A:ILE:HA | 1:99:A:VAL:HB | 3 | 0.34 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 2 | 0.34 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 2 | 0.34 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 2 | 0.34 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 16 | 0.34 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 16 | 0.34 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 16 | 0.34 |
| (1,778) | 1:8:A:ILE:HG21 | 1:13:A:LEU:HD21 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG21 | 1:13:A:LEU:HD22 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG21 | 1:13:A:LEU:HD23 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG22 | 1:13:A:LEU:HD21 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG22 | 1:13:A:LEU:HD22 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG22 | 1:13:A:LEU:HD23 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG23 | 1:13:A:LEU:HD21 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG23 | 1:13:A:LEU:HD22 | 6 | 0.34 |
| (1,778) | 1:8:A:ILE:HG23 | 1:13:A:LEU:HD23 | 6 | 0.34 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 8 | 0.34 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 13 | 0.34 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 13 | 0.34 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 20 | 0.34 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 20 | 0.34 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 20 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 20 | 0.34 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 20 | 0.34 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 20 | 0.34 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 15 | 0.34 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 17 | 0.34 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 2 | 0.34 |
| (1,285) | 1:9:A:ASN:HB2 | 1:12:A:MET:H | 10 | 0.34 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 11 | 0.34 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 16 | 0.34 |
| (1,234) | 1:10:A:PRO:HA | 1:28:A:PHE:H | 8 | 0.34 |
| (1,229) | 1:213:A:ARG:H | 1:214:A:PHE:HA | 7 | 0.34 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 18 | 0.34 |
| (1,193) | 1:192:A:THR:HA | 1:196:A:ASP:H | 5 | 0.34 |
| (1,122) | 1:99:A:VAL:HG11 | 1:102:A:ASN:H | 9 | 0.34 |
| (1,122) | 1:99:A:VAL:HG12 | 1:102:A:ASN:H | 9 | 0.34 |
| (1,122) | 1:99:A:VAL:HG13 | 1:102:A:ASN:H | 9 | 0.34 |
| (1,122) | 1:99:A:VAL:HG21 | 1:102:A:ASN:H | 9 | 0.34 |
| (1,122) | 1:99:A:VAL:HG22 | 1:102:A:ASN:H | 9 | 0.34 |
| (1,122) | 1:99:A:VAL:HG23 | 1:102:A:ASN:H | 9 | 0.34 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 3 | 0.34 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 3 | 0.34 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 3 | 0.34 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 3 | 0.34 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 3 | 0.34 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 3 | 0.34 |
| (1,52) | 1:32:A:LEU:H | 1:32:A:LEU:HG | 14 | 0.34 |
| (1,2357) | 1:211:A:GLU:H | 1:211:A:GLU:HB2 | 5 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 2 | 0.33 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 2 | 0.33 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE21 | 20 | 0.33 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE22 | 20 | 0.33 |
| (1,1965) | 1:49:A:LEU:HD11 | 1:219:A:LEU:H | 10 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1965) | 1:49:A:LEU:HD12 | 1:219:A:LEU:H | 10 | 0.33 |
| (1,1965) | 1:49:A:LEU:HD13 | 1:219:A:LEU:H | 10 | 0.33 |
| (1,1965) | 1:49:A:LEU:HD21 | 1:219:A:LEU:H | 10 | 0.33 |
| (1,1965) | 1:49:A:LEU:HD22 | 1:219:A:LEU:H | 10 | 0.33 |
| (1,1965) | 1:49:A:LEU:HD23 | 1:219:A:LEU:H | 10 | 0.33 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 19 | 0.33 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 19 | 0.33 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 19 | 0.33 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 19 | 0.33 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 19 | 0.33 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 19 | 0.33 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 7 | 0.33 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 14 | 0.33 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 17 | 0.33 |
| (1,1650) | 1:153:A:ARG:H | 1:153:A:ARG:HG2 | 14 | 0.33 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 15 | 0.33 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 7 | 0.33 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 5 | 0.33 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 5 | 0.33 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 5 | 0.33 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 7 | 0.33 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 6 | 0.33 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 11 | 0.33 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 17 | 0.33 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 17 | 0.33 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 17 | 0.33 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 17 | 0.33 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD11 | 19 | 0.33 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD12 | 19 | 0.33 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD13 | 19 | 0.33 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD21 | 19 | 0.33 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD22 | 19 | 0.33 |
| (1,1280) | 1:50:A:LEU:HB2 | 1:164:A:LEU:HD23 | 19 | 0.33 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 17 | 0.33 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 11 | 0.33 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 11 | 0.33 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 11 | 0.33 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 11 | 0.33 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 11 | 0.33 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 11 | 0.33 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 6 | 0.33 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 6 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 1 | 0.33 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 3 | 0.33 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 9 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG21 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG22 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG23 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG21 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG22 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG23 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG21 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG22 | 3 | 0.33 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG23 | 3 | 0.33 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 5 | 0.33 |
| (1,976) | 1:82:A:MET:HE1 | 1:93:A:ILE:H | 1 | 0.33 |
| (1,976) | 1:82:A:MET:HE2 | 1:93:A:ILE:H | 1 | 0.33 |
| (1,976) | 1:82:A:MET:HE3 | 1:93:A:ILE:H | 1 | 0.33 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE1 | 14 | 0.33 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE2 | 14 | 0.33 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE3 | 14 | 0.33 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 4 | 0.33 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 4 | 0.33 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 4 | 0.33 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 1 | 0.33 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 1 | 0.33 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 1 | 0.33 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 10 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 10 | 0.33 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 10 | 0.33 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 10 | 0.33 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 10 | 0.33 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 10 | 0.33 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 11 | 0.33 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 6 | 0.33 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 16 | 0.33 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 16 | 0.33 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 16 | 0.33 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 16 | 0.33 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 16 | 0.33 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 16 | 0.33 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 14 | 0.33 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 10 | 0.33 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 13 | 0.33 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 1 | 0.33 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 1 | 0.33 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 1 | 0.33 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 6 | 0.33 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 7 | 0.33 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 20 | 0.33 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 19 | 0.33 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 7 | 0.32 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 7 | 0.32 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 7 | 0.32 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 7 | 0.32 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 7 | 0.32 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 7 | 0.32 |
| (1,2302) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HA | 12 | 0.32 |
| (1,2302) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HA | 12 | 0.32 |
| (1,2302) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HA | 12 | 0.32 |
| (1,2302) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HA | 12 | 0.32 |
| (1,2302) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HA | 12 | 0.32 |
| (1,2302) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HA | 12 | 0.32 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 9 | 0.32 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 9 | 0.32 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 9 | 0.32 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 9 | 0.32 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 9 | 0.32 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 9 | 0.32 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 14 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 14 | 0.32 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 14 | 0.32 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 14 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 9 | 0.32 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 9 | 0.32 |
| (1,2193) | 1:131:A:LYS:H | 1:132:A:CYS:HB2 | 12 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 1 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 1 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 1 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 1 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 1 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 1 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 14 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 14 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 14 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 14 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 14 | 0.32 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 14 | 0.32 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD1 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD2 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD1 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD2 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD1 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD2 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD1 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD2 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD1 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD2 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD1 | 1 | 0.32 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD2 | 1 | 0.32 |
| (1,1831) | 1:7:A:GLU:HG2 | 1:8:A:ILE:HG12 | 12 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 18 | 0.32 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 17 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB1 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB2 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB3 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB1 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB2 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB3 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB1 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB2 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB3 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB1 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB2 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB3 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB1 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB2 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB3 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB1 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB2 | 11 | 0.32 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB3 | 11 | 0.32 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 8 | 0.32 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 8 | 0.32 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 8 | 0.32 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 3 | 0.32 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 3 | 0.32 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 3 | 0.32 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 5 | 0.32 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 12 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 6 | 0.32 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 6 | 0.32 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD1 | 18 | 0.32 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD2 | 18 | 0.32 |
| (1,1157) | 1:28:A:PHE:HA | 1:217:A:VAL:HA | 9 | 0.32 |
| (1,1152) | 1:165:A:PHE:HD1 | 1:174:A:GLU:HA | 12 | 0.32 |
| (1,1152) | 1:165:A:PHE:HD2 | 1:174:A:GLU:HA | 12 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 2 | 0.32 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 14 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 12 | 0.32 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 12 | 0.32 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 7 | 0.32 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 7 | 0.32 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 7 | 0.32 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 10 | 0.32 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 10 | 0.32 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 10 | 0.32 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 5 | 0.32 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 16 | 0.32 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 4 | 0.32 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 18 | 0.32 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 6 | 0.32 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 13 | 0.32 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 14 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 2 | 0.32 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 2 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD11 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD12 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD13 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD11 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD12 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD13 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD11 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD12 | 16 | 0.32 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD13 | 16 | 0.32 |
| (1,844) | 1:132:A:CYS:HA | 1:135:A:LYS:HE2 | 3 | 0.32 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 9 | 0.32 |
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 9 | 0.32 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 9 | 0.32 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 17 | 0.32 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 17 | 0.32 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 14 | 0.32 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 17 | 0.32 |
| (1,557) | 1:74:A:GLU:HB2 | 1:75:A:VAL:H | 14 | 0.32 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 18 | 0.32 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 3 | 0.32 |
| (1,297) | 1:159:A:ASN:HA | 1:160:A:PHE:H | 1 | 0.32 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 7 | 0.32 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 7 | 0.32 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 15 | 0.32 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 20 | 0.31 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 20 | 0.31 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 20 | 0.31 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 20 | 0.31 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 20 | 0.31 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 20 | 0.31 |
| (1,2290) | 1:168:A:VAL:HG11 | 1:169:A:ASP:HA | 15 | 0.31 |
| (1,2290) | 1:168:A:VAL:HG12 | 1:169:A:ASP:HA | 15 | 0.31 |
| (1,2290) | 1:168:A:VAL:HG13 | 1:169:A:ASP:HA | 15 | 0.31 |
| (1,2290) | 1:168:A:VAL:HG21 | 1:169:A:ASP:HA | 15 | 0.31 |
| (1,2290) | 1:168:A:VAL:HG22 | 1:169:A:ASP:HA | 15 | 0.31 |
| (1,2290) | 1:168:A:VAL:HG23 | 1:169:A:ASP:HA | 15 | 0.31 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 10 | 0.31 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 10 | 0.31 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 18 | 0.31 |
| (1,2192) | 1:129:A:ARG:HG2 | 1:132:A:CYS:HB2 | 15 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 19 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 19 | 0.31 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 19 | 0.31 |
| (1,2031) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HA | 11 | 0.31 |
| (1,2031) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HA | 11 | 0.31 |
| (1,2031) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HA | 11 | 0.31 |
| (1,2031) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HA | 11 | 0.31 |
| (1,2031) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HA | 11 | 0.31 |
| (1,2031) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HA | 11 | 0.31 |
| (1,1996) | 1:55:A:LEU:HD11 | 1:160:A:PHE:HA | 18 | 0.31 |
| (1,1996) | 1:55:A:LEU:HD12 | 1:160:A:PHE:HA | 18 | 0.31 |
| (1,1996) | 1:55:A:LEU:HD13 | 1:160:A:PHE:HA | 18 | 0.31 |
| (1,1996) | 1:55:A:LEU:HD21 | 1:160:A:PHE:HA | 18 | 0.31 |
| (1,1996) | 1:55:A:LEU:HD22 | 1:160:A:PHE:HA | 18 | 0.31 |
| (1,1996) | 1:55:A:LEU:HD23 | 1:160:A:PHE:HA | 18 | 0.31 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD11 | 16 | 0.31 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD12 | 16 | 0.31 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD13 | 16 | 0.31 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD21 | 16 | 0.31 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD22 | 16 | 0.31 |
| (1,1915) | 1:31:A:VAL:HA | 1:32:A:LEU:HD23 | 16 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 17 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 17 | 0.31 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 17 | 0.31 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 16 | 0.31 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 12 | 0.31 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 17 | 0.31 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 2 | 0.31 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG11 | 1 | 0.31 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG12 | 1 | 0.31 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG13 | 1 | 0.31 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG21 | 1 | 0.31 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG22 | 1 | 0.31 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG23 | 1 | 0.31 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 3 | 0.31 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 20 | 0.31 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 6 | 0.31 |
| (1,1721) | 1:225:A:GLU:HG2 | 1:226:A:HIS:H | 16 | 0.31 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 1 | 0.31 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 1 | 0.31 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 1 | 0.31 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 10 | 0.31 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 4 | 0.31 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 11 | 0.31 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 11 | 0.31 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 11 | 0.31 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 11 | 0.31 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 11 | 0.31 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 11 | 0.31 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD1 | 5 | 0.31 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD2 | 5 | 0.31 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD1 | 5 | 0.31 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD2 | 5 | 0.31 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD1 | 5 | 0.31 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD2 | 5 | 0.31 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 20 | 0.31 |
| (1,1428) | 1:23:A:ALA:HB1 | 1:107:A:GLY:HA2 | 16 | 0.31 |
| (1,1428) | 1:23:A:ALA:HB2 | 1:107:A:GLY:HA2 | 16 | 0.31 |
| (1,1428) | 1:23:A:ALA:HB3 | 1:107:A:GLY:HA2 | 16 | 0.31 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 19 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG11 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG12 | 13 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG13 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG21 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG22 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG23 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG11 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG12 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG13 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG21 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG22 | 13 | 0.31 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG23 | 13 | 0.31 |
| (1,1238) | 1:55:A:LEU:HG | 1:160:A:PHE:HA | 12 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD11 | 11 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD12 | 11 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD13 | 11 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD11 | 11 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD12 | 11 | 0.31 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD13 | 11 | 0.31 |
| (1,1052) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE21 | 8 | 0.31 |
| (1,1052) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE21 | 8 | 0.31 |
| (1,1052) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE21 | 8 | 0.31 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 11 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG21 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG22 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG23 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG21 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG22 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG23 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG21 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG22 | 9 | 0.31 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG23 | 9 | 0.31 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE1 | 14 | 0.31 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE2 | 14 | 0.31 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE3 | 14 | 0.31 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE1 | 14 | 0.31 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE2 | 14 | 0.31 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE3 | 14 | 0.31 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 15 | 0.31 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 15 | 0.31 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 15 | 0.31 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 15 | 0.31 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 15 | 0.31 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 15 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 6 | 0.31 |
| (1,858) | 1:151:A:GLN:H | 1:151:A:GLN:HG2 | 2 | 0.31 |
| (1,829) | 1:113:A:VAL:HA | 1:115:A:LYS:HB2 | 16 | 0.31 |
| (1,766) | 1:134:A:GLU:HA | 1:140:A:GLN:HE22 | 10 | 0.31 |
| (1,765) | 1:192:A:THR:HA | 1:194:A:LEU:H | 11 | 0.31 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 18 | 0.31 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 15 | 0.31 |
| (1,739) | 1:163:A:ILE:HB | 1:177:A:GLY:H | 20 | 0.31 |
| (1,731) | 1:194:A:LEU:H | 1:196:A:ASP:H | 9 | 0.31 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 5 | 0.31 |
| (1,574) | 1:164:A:LEU:HG | 1:175:A:LEU:H | 13 | 0.31 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 12 | 0.31 |
| (1,502) | 1:224:A:LEU:HG | 1:225:A:GLU:H | 16 | 0.31 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 14 | 0.31 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 18 | 0.31 |
| (1,358) | 1:127:A:GLU:H | 1:128:A:ASP:HB2 | 15 | 0.31 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 9 | 0.31 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 9 | 0.31 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 9 | 0.31 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 18 | 0.31 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 18 | 0.31 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 18 | 0.31 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 20 | 0.31 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 1 | 0.31 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 1 | 0.31 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 1 | 0.31 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 1 | 0.31 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 1 | 0.31 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 1 | 0.31 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE21 | 3 | 0.3 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE22 | 3 | 0.3 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE21 | 18 | 0.3 |
| (1,2355) | 1:209:A:GLN:H | 1:209:A:GLN:HE22 | 18 | 0.3 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 10 | 0.3 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 10 | 0.3 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 10 | 0.3 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 10 | 0.3 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 10 | 0.3 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 10 | 0.3 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 11 | 0.3 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 11 | 0.3 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 11 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 11 | 0.3 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 11 | 0.3 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 11 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD11 | 15 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD12 | 15 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD13 | 15 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD21 | 15 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD22 | 15 | 0.3 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD23 | 15 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 16 | 0.3 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 16 | 0.3 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 1 | 0.3 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 1 | 0.3 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 1 | 0.3 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 19 | 0.3 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 19 | 0.3 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 19 | 0.3 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 19 | 0.3 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 19 | 0.3 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 19 | 0.3 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 20 | 0.3 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 4 | 0.3 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 4 | 0.3 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 4 | 0.3 |
| (1,1724) | 1:74:A:GLU:HG2 | 1:75:A:VAL:H | 13 | 0.3 |
| (1,1718) | 1:210:A:GLY:H | 1:211:A:GLU:HG2 | 12 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 9 | 0.3 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 12 | 0.3 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 12 | 0.3 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 12 | 0.3 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 12 | 0.3 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 12 | 0.3 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 12 | 0.3 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE1 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE2 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE3 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE1 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE2 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE3 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE1 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE2 | 1 | 0.3 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE3 | 1 | 0.3 |
| (1,1476) | 1:153:A:ARG:H | 1:153:A:ARG:HD2 | 1 | 0.3 |
| (1,1465) | 1:212:A:VAL:HB | 1:213:A:ARG:HD2 | 8 | 0.3 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 1 | 0.3 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 4 | 0.3 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 14 | 0.3 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 14 | 0.3 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 14 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 17 | 0.3 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 17 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG11 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG12 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG13 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG21 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG22 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG23 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG11 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG12 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG13 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG21 | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG22 | 16 | 0.3 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG23 | 16 | 0.3 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 15 | 0.3 |
| (1,1238) | 1:55:A:LEU:HG | 1:160:A:PHE:HA | 15 | 0.3 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG11 | 15 | 0.3 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG12 | 15 | 0.3 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG13 | 15 | 0.3 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG21 | 15 | 0.3 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG22 | 15 | 0.3 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG23 | 15 | 0.3 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 14 | 0.3 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 18 | 0.3 |
| (1,1131) | 1:106:A:LEU:HG | 1:108:A:PHE:HE1 | 3 | 0.3 |
| (1,1131) | 1:106:A:LEU:HG | 1:108:A:PHE:HE2 | 3 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG21 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG22 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG23 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG21 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG22 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG23 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG21 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG22 | 10 | 0.3 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG23 | 10 | 0.3 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD11 | 15 | 0.3 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD12 | 15 | 0.3 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD13 | 15 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 8 | 0.3 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 8 | 0.3 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 1 | 0.3 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 1 | 0.3 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 1 | 0.3 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 10 | 0.3 |
| (1,1046) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 11 | 0.3 |
| (1,1046) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 11 | 0.3 |
| (1,1046) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 11 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 6 | 0.3 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 10 | 0.3 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 14 | 0.3 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 15 | 0.3 |
| (1,971) | 1:12:A:MET:HE1 | 1:150:A:GLY:H | 14 | 0.3 |
| (1,971) | 1:12:A:MET:HE2 | 1:150:A:GLY:H | 14 | 0.3 |
| (1,971) | 1:12:A:MET:HE3 | 1:150:A:GLY:H | 14 | 0.3 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 9 | 0.3 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 9 | 0.3 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 9 | 0.3 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 10 | 0.3 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD1 | 18 | 0.3 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD2 | 18 | 0.3 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 20 | 0.3 |
| (1,622) | 1:80:A:TYR:HE1 | 1:121:A:THR:H | 13 | 0.3 |
| (1,576) | 1:171:A:HIS:HD2 | 1:172:A:LEU:H | 12 | 0.3 |
| (1,557) | 1:74:A:GLU:HB2 | 1:75:A:VAL:H | 8 | 0.3 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD11 | 7 | 0.3 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD12 | 7 | 0.3 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD13 | 7 | 0.3 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 2 | 0.3 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 2 | 0.3 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 2 | 0.3 |
| (1,368) | 1:18:A:TYR:H | 1:19:A:ARG:HB2 | 17 | 0.3 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 3 | 0.3 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 9 | 0.3 |
| (1,361) | 1:15:A:LYS:H | 1:15:A:LYS:HE2 | 1 | 0.3 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 5 | 0.3 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 12 | 0.3 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 12 | 0.3 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 12 | 0.3 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 18 | 0.3 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 3 | 0.3 |
| (1,80) | 1:52:A:LEU:H | 1:53:A:PHE:HD1 | 15 | 0.3 |
| (1,80) | 1:52:A:LEU:H | 1:53:A:PHE:HD2 | 15 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 13 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 13 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 13 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 13 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 13 | 0.3 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 13 | 0.3 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 10 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 15 | 0.29 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 15 | 0.29 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 15 | 0.29 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 3 | 0.29 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 3 | 0.29 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 3 | 0.29 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 3 | 0.29 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 3 | 0.29 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 3 | 0.29 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 18 | 0.29 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 18 | 0.29 |
| (1,2196) | 1:134:A:GLU:HB2 | 1:140:A:GLN:HE21 | 10 | 0.29 |
| (1,2196) | 1:134:A:GLU:HB2 | 1:140:A:GLN:HE22 | 10 | 0.29 |
| (1,1969) | 1:51:A:LEU:HD11 | 1:52:A:LEU:HA | 17 | 0.29 |
| (1,1969) | 1:51:A:LEU:HD12 | 1:52:A:LEU:HA | 17 | 0.29 |
| (1,1969) | 1:51:A:LEU:HD13 | 1:52:A:LEU:HA | 17 | 0.29 |
| (1,1969) | 1:51:A:LEU:HD21 | 1:52:A:LEU:HA | 17 | 0.29 |
| (1,1969) | 1:51:A:LEU:HD22 | 1:52:A:LEU:HA | 17 | 0.29 |
| (1,1969) | 1:51:A:LEU:HD23 | 1:52:A:LEU:HA | 17 | 0.29 |
| (1,1917) | 1:32:A:LEU:H | 1:32:A:LEU:HD11 | 10 | 0.29 |
| (1,1917) | 1:32:A:LEU:H | 1:32:A:LEU:HD12 | 10 | 0.29 |
| (1,1917) | 1:32:A:LEU:H | 1:32:A:LEU:HD13 | 10 | 0.29 |
| (1,1917) | 1:32:A:LEU:H | 1:32:A:LEU:HD21 | 10 | 0.29 |
| (1,1917) | 1:32:A:LEU:H | 1:32:A:LEU:HD22 | 10 | 0.29 |
| (1,1917) | 1:32:A:LEU:H | 1:32:A:LEU:HD23 | 10 | 0.29 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 14 | 0.29 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 14 | 0.29 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 14 | 0.29 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 14 | 0.29 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 14 | 0.29 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 14 | 0.29 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 5 | 0.29 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE1 | 3 | 0.29 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE2 | 3 | 0.29 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE3 | 3 | 0.29 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 20 | 0.29 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 20 | 0.29 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 20 | 0.29 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 1 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 1 | 0.29 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 1 | 0.29 |
| (1,1639) | 1:19:A:ARG:H | 1:20:A:LEU:HB2 | 15 | 0.29 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 8 | 0.29 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 8 | 0.29 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 8 | 0.29 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 4 | 0.29 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 15 | 0.29 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 4 | 0.29 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 11 | 0.29 |
| (1,1410) | 1:137:A:GLU:H | 1:140:A:GLN:HB2 | 18 | 0.29 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 12 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 13 | 0.29 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 13 | 0.29 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 12 | 0.29 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 4 | 0.29 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 4 | 0.29 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 4 | 0.29 |
| (1,1080) | 1:8:A:ILE:HG12 | 1:90:A:CYS:HA | 11 | 0.29 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 13 | 0.29 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 13 | 0.29 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 13 | 0.29 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 16 | 0.29 |
| (1,1045) | 1:67:A:ILE:HA | 1:70:A:LEU:HB2 | 19 | 0.29 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 5 | 0.29 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 7 | 0.29 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 12 | 0.29 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 20 | 0.29 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 9 | 0.29 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 9 | 0.29 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 9 | 0.29 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 7 | 0.29 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 7 | 0.29 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD11 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD12 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG21 | 1:96:A:ILE:HD13 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD11 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD12 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG22 | 1:96:A:ILE:HD13 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD11 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD12 | 6 | 0.29 |
| (1,895) | 1:96:A:ILE:HG23 | 1:96:A:ILE:HD13 | 6 | 0.29 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG21 | 19 | 0.29 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG22 | 19 | 0.29 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG23 | 19 | 0.29 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 11 | 0.29 |
| (1,637) | 1:176:A:ASP:H | 1:183:A:VAL:H | 10 | 0.29 |
| (1,582) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD21 | 4 | 0.29 |
| (1,582) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD21 | 4 | 0.29 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 10 | 0.29 |
| (1,443) | 1:135:A:LYS:H | 1:135:A:LYS:HE2 | 2 | 0.29 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 2 | 0.29 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 12 | 0.29 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 14 | 0.29 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 14 | 0.29 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 14 | 0.29 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 20 | 0.29 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,168) | 1:157:A:LYS:HG2 | 1:158:A:VAL:H | 2 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 4 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 4 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 4 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 4 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 4 | 0.29 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 4 | 0.29 |
| (1,23) | 1:34:A:LEU:H | 1:34:A:LEU:HG | 14 | 0.29 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 9 | 0.28 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 9 | 0.28 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 9 | 0.28 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 9 | 0.28 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 9 | 0.28 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 9 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 2 | 0.28 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 2 | 0.28 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 18 | 0.28 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 18 | 0.28 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 18 | 0.28 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 18 | 0.28 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 18 | 0.28 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 18 | 0.28 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 16 | 0.28 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 16 | 0.28 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 16 | 0.28 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 16 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 16 | 0.28 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 16 | 0.28 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG11 | 7 | 0.28 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG12 | 7 | 0.28 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG13 | 7 | 0.28 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG21 | 7 | 0.28 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG22 | 7 | 0.28 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG23 | 7 | 0.28 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE21 | 18 | 0.28 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE22 | 18 | 0.28 |
| (1,2033) | 1:70:A:LEU:HD11 | 1:185:A:HIS:H | 11 | 0.28 |
| (1,2033) | 1:70:A:LEU:HD12 | 1:185:A:HIS:H | 11 | 0.28 |
| (1,2033) | 1:70:A:LEU:HD13 | 1:185:A:HIS:H | 11 | 0.28 |
| (1,2033) | 1:70:A:LEU:HD21 | 1:185:A:HIS:H | 11 | 0.28 |
| (1,2033) | 1:70:A:LEU:HD22 | 1:185:A:HIS:H | 11 | 0.28 |
| (1,2033) | 1:70:A:LEU:HD23 | 1:185:A:HIS:H | 11 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HD21 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HD22 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HD21 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HD22 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HD21 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HD22 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HD21 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HD22 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HD21 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HD22 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HD21 | 10 | 0.28 |
| (1,2032) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HD22 | 10 | 0.28 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 8 | 0.28 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 14 | 0.28 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 9 | 0.28 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 9 | 0.28 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 9 | 0.28 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 9 | 0.28 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 9 | 0.28 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 9 | 0.28 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 4 | 0.28 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 16 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 15 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 15 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 15 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 15 | 0.28 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 15 | 0.28 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 7 | 0.28 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 7 | 0.28 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 7 | 0.28 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 4 | 0.28 |
| (1,1804) | 1:3:A:LEU:HD11 | 1:4:A:LYS:H | 12 | 0.28 |
| (1,1804) | 1:3:A:LEU:HD12 | 1:4:A:LYS:H | 12 | 0.28 |
| (1,1804) | 1:3:A:LEU:HD13 | 1:4:A:LYS:H | 12 | 0.28 |
| (1,1804) | 1:3:A:LEU:HD21 | 1:4:A:LYS:H | 12 | 0.28 |
| (1,1804) | 1:3:A:LEU:HD22 | 1:4:A:LYS:H | 12 | 0.28 |
| (1,1804) | 1:3:A:LEU:HD23 | 1:4:A:LYS:H | 12 | 0.28 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 9 | 0.28 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 9 | 0.28 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 9 | 0.28 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 10 | 0.28 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 15 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 12 | 0.28 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 12 | 0.28 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 20 | 0.28 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 1 | 0.28 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 1 | 0.28 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 2 | 0.28 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 6 | 0.28 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 12 | 0.28 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 12 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 12 | 0.28 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 2 | 0.28 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 5 | 0.28 |
| (1,1243) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD11 | 5 | 0.28 |
| (1,1243) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD12 | 5 | 0.28 |
| (1,1243) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD13 | 5 | 0.28 |
| (1,1233) | 1:154:A:VAL:HA | 1:156:A:ASP:HB2 | 13 | 0.28 |
| (1,1189) | 1:34:A:LEU:H | 1:38:A:SER:HB2 | 1 | 0.28 |
| (1,1184) | 1:172:A:LEU:H | 1:188:A:SER:HB2 | 15 | 0.28 |
| (1,1152) | 1:165:A:PHE:HD1 | 1:174:A:GLU:HA | 15 | 0.28 |
| (1,1152) | 1:165:A:PHE:HD2 | 1:174:A:GLU:HA | 15 | 0.28 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 14 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 11 | 0.28 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 11 | 0.28 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 9 | 0.28 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 9 | 0.28 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 9 | 0.28 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 5 | 0.28 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 5 | 0.28 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 5 | 0.28 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 18 | 0.28 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 18 | 0.28 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 18 | 0.28 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 5 | 0.28 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 6 | 0.28 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 10 | 0.28 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 10 | 0.28 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 10 | 0.28 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 2 | 0.28 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 19 | 0.28 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 1 | 0.28 |
| (1,1007) | 1:17:A:LEU:HA | 1:17:A:LEU:HG | 17 | 0.28 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD21 | 10 | 0.28 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD22 | 10 | 0.28 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD23 | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 8 | 0.28 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 8 | 0.28 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 13 | 0.28 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 13 | 0.28 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 13 | 0.28 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 13 | 0.28 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 13 | 0.28 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 13 | 0.28 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 9 | 0.28 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 9 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 11 | 0.28 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 3 | 0.28 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 3 | 0.28 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 3 | 0.28 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 1 | 0.28 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG21 | 3 | 0.28 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG22 | 3 | 0.28 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG23 | 3 | 0.28 |
| (1,801) | 1:56:A:THR:HG21 | 1:57:A:ALA:HA | 20 | 0.28 |
| (1,801) | 1:56:A:THR:HG22 | 1:57:A:ALA:HA | 20 | 0.28 |
| (1,801) | 1:56:A:THR:HG23 | 1:57:A:ALA:HA | 20 | 0.28 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 2 | 0.28 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 2 | 0.28 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 2 | 0.28 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 10 | 0.28 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 5 | 0.28 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 18 | 0.28 |
| (1,518) | 1:3:A:LEU:H | 1:87:A:GLY:H | 13 | 0.28 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 19 | 0.28 |
| (1,403) | 1:99:A:VAL:HG11 | 1:103:A:GLN:HE21 | 5 | 0.28 |
| (1,403) | 1:99:A:VAL:HG12 | 1:103:A:GLN:HE21 | 5 | 0.28 |
| (1,403) | 1:99:A:VAL:HG13 | 1:103:A:GLN:HE21 | 5 | 0.28 |
| (1,403) | 1:99:A:VAL:HG21 | 1:103:A:GLN:HE21 | 5 | 0.28 |
| (1,403) | 1:99:A:VAL:HG22 | 1:103:A:GLN:HE21 | 5 | 0.28 |
| (1,403) | 1:99:A:VAL:HG23 | 1:103:A:GLN:HE21 | 5 | 0.28 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 4 | 0.28 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 11 | 0.28 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 10 | 0.28 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 3 | 0.28 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 3 | 0.28 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 3 | 0.28 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG21 | 3 | 0.28 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG22 | 3 | 0.28 |
| (1,308) | 1:76:A:SER:H | 1:79:A:VAL:HG23 | 3 | 0.28 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 13 | 0.28 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 4 | 0.28 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 1 | 0.28 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 12 | 0.28 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 15 | 0.28 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 1 | 0.28 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 7 | 0.28 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 9 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 13 | 0.27 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 13 | 0.27 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 13 | 0.27 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 13 | 0.27 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 13 | 0.27 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 13 | 0.27 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 11 | 0.27 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 11 | 0.27 |
| (1,2175) | 1:118:A:LEU:HD11 | 1:122:A:GLU:HA | 7 | 0.27 |
| (1,2175) | 1:118:A:LEU:HD12 | 1:122:A:GLU:HA | 7 | 0.27 |
| (1,2175) | 1:118:A:LEU:HD13 | 1:122:A:GLU:HA | 7 | 0.27 |
| (1,2175) | 1:118:A:LEU:HD21 | 1:122:A:GLU:HA | 7 | 0.27 |
| (1,2175) | 1:118:A:LEU:HD22 | 1:122:A:GLU:HA | 7 | 0.27 |
| (1,2175) | 1:118:A:LEU:HD23 | 1:122:A:GLU:HA | 7 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 12 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 13 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 13 | 0.27 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 13 | 0.27 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD11 | 13 | 0.27 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD12 | 13 | 0.27 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD13 | 13 | 0.27 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD21 | 13 | 0.27 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD22 | 13 | 0.27 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD23 | 13 | 0.27 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 16 | 0.27 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 16 | 0.27 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 16 | 0.27 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 16 | 0.27 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 16 | 0.27 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 16 | 0.27 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 20 | 0.27 |
| (1,1962) | 1:49:A:LEU:HD11 | 1:198:A:ALA:HA | 20 | 0.27 |
| (1,1962) | 1:49:A:LEU:HD12 | 1:198:A:ALA:HA | 20 | 0.27 |
| (1,1962) | 1:49:A:LEU:HD13 | 1:198:A:ALA:HA | 20 | 0.27 |
| (1,1962) | 1:49:A:LEU:HD21 | 1:198:A:ALA:HA | 20 | 0.27 |
| (1,1962) | 1:49:A:LEU:HD22 | 1:198:A:ALA:HA | 20 | 0.27 |
| (1,1962) | 1:49:A:LEU:HD23 | 1:198:A:ALA:HA | 20 | 0.27 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD11 | 7 | 0.27 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD12 | 7 | 0.27 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD13 | 7 | 0.27 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD21 | 7 | 0.27 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD22 | 7 | 0.27 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD23 | 7 | 0.27 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 14 | 0.27 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD11 | 5 | 0.27 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD12 | 5 | 0.27 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD13 | 5 | 0.27 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD21 | 5 | 0.27 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD22 | 5 | 0.27 |
| (1,1924) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HD23 | 5 | 0.27 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 20 | 0.27 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 17 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 17 | 0.27 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 17 | 0.27 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 17 | 0.27 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 17 | 0.27 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 17 | 0.27 |
| (1,1848) | 1:13:A:LEU:HA | 1:17:A:LEU:HB2 | 16 | 0.27 |
| (1,1831) | 1:7:A:GLU:HG2 | 1:8:A:ILE:HG12 | 10 | 0.27 |
| (1,1761) | 1:85:A:THR:HA | 1:86:A:ILE:HB | 1 | 0.27 |
| (1,1721) | 1:225:A:GLU:HG2 | 1:226:A:HIS:H | 4 | 0.27 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 8 | 0.27 |
| (1,1622) | 1:51:A:LEU:HD11 | 1:53:A:PHE:HB2 | 17 | 0.27 |
| (1,1622) | 1:51:A:LEU:HD12 | 1:53:A:PHE:HB2 | 17 | 0.27 |
| (1,1622) | 1:51:A:LEU:HD13 | 1:53:A:PHE:HB2 | 17 | 0.27 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 13 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 18 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 18 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 18 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 18 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 18 | 0.27 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 18 | 0.27 |
| (1,1428) | 1:23:A:ALA:HB1 | 1:107:A:GLY:HA2 | 5 | 0.27 |
| (1,1428) | 1:23:A:ALA:HB2 | 1:107:A:GLY:HA2 | 5 | 0.27 |
| (1,1428) | 1:23:A:ALA:HB3 | 1:107:A:GLY:HA2 | 5 | 0.27 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 20 | 0.27 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 18 | 0.27 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 1 | 0.27 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 18 | 0.27 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 11 | 0.27 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 11 | 0.27 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 11 | 0.27 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 13 | 0.27 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 13 | 0.27 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 14 | 0.27 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 14 | 0.27 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 17 | 0.27 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 17 | 0.27 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 13 | 0.27 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 8 | 0.27 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 8 | 0.27 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 8 | 0.27 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 11 | 0.27 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 11 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 11 | 0.27 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 15 | 0.27 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 15 | 0.27 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 15 | 0.27 |
| (1,1080) | 1:8:A:ILE:HG12 | 1:90:A:CYS:HA | 16 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 12 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 12 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 12 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 14 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 14 | 0.27 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 14 | 0.27 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 3 | 0.27 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 19 | 0.27 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 4 | 0.27 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 4 | 0.27 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 4 | 0.27 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 12 | 0.27 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 17 | 0.27 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 3 | 0.27 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 8 | 0.27 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 11 | 0.27 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD11 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD12 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE1 | 1:93:A:ILE:HD13 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD11 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD12 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE2 | 1:93:A:ILE:HD13 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD11 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD12 | 15 | 0.27 |
| (1,975) | 1:82:A:MET:HE3 | 1:93:A:ILE:HD13 | 15 | 0.27 |
| (1,900) | 1:172:A:LEU:HG | 1:188:A:SER:HB2 | 19 | 0.27 |
| (1,889) | 1:171:A:HIS:HD2 | 1:187:A:ALA:HA | 2 | 0.27 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 18 | 0.27 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 9 | 0.27 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 9 | 0.27 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 9 | 0.27 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 4 | 0.27 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 4 | 0.27 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 4 | 0.27 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 18 | 0.27 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 18 | 0.27 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,761) | 1:49:A:LEU:H | 1:165:A:PHE:HD1 | 10 | 0.27 |
| (1,761) | 1:49:A:LEU:H | 1:165:A:PHE:HD2 | 10 | 0.27 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 4 | 0.27 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 4 | 0.27 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 4 | 0.27 |
| (1,727) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE22 | 3 | 0.27 |
| (1,727) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE22 | 3 | 0.27 |
| (1,727) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE22 | 3 | 0.27 |
| (1,632) | 1:34:A:LEU:HD11 | 1:35:A:GLU:H | 15 | 0.27 |
| (1,632) | 1:34:A:LEU:HD12 | 1:35:A:GLU:H | 15 | 0.27 |
| (1,632) | 1:34:A:LEU:HD13 | 1:35:A:GLU:H | 15 | 0.27 |
| (1,632) | 1:34:A:LEU:HD21 | 1:35:A:GLU:H | 15 | 0.27 |
| (1,632) | 1:34:A:LEU:HD22 | 1:35:A:GLU:H | 15 | 0.27 |
| (1,632) | 1:34:A:LEU:HD23 | 1:35:A:GLU:H | 15 | 0.27 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 9 | 0.27 |
| (1,590) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 17 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 11 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 11 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 11 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 11 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 11 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 11 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 12 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 12 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 12 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 12 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 12 | 0.27 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 12 | 0.27 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 9 | 0.27 |
| (1,467) | 1:171:A:HIS:H | 1:173:A:TYR:HE1 | 1 | 0.27 |
| (1,467) | 1:171:A:HIS:H | 1:173:A:TYR:HE2 | 1 | 0.27 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 16 | 0.27 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 19 | 0.27 |
| (1,358) | 1:127:A:GLU:H | 1:128:A:ASP:HB2 | 11 | 0.27 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD1 | 6 | 0.27 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD2 | 6 | 0.27 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 11 | 0.27 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 11 | 0.27 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 11 | 0.27 |
| (1,314) | 1:188:A:SER:HB2 | 1:193:A:LEU:H | 9 | 0.27 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 14 | 0.27 |
| (1,193) | 1:192:A:THR:HA | 1:196:A:ASP:H | 12 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 11 | 0.27 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 11 | 0.27 |
| (1,122) | 1:99:A:VAL:HG11 | 1:102:A:ASN:H | 19 | 0.27 |
| (1,122) | 1:99:A:VAL:HG12 | 1:102:A:ASN:H | 19 | 0.27 |
| (1,122) | 1:99:A:VAL:HG13 | 1:102:A:ASN:H | 19 | 0.27 |
| (1,122) | 1:99:A:VAL:HG21 | 1:102:A:ASN:H | 19 | 0.27 |
| (1,122) | 1:99:A:VAL:HG22 | 1:102:A:ASN:H | 19 | 0.27 |
| (1,122) | 1:99:A:VAL:HG23 | 1:102:A:ASN:H | 19 | 0.27 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 3 | 0.27 |
| (1,52) | 1:32:A:LEU:H | 1:32:A:LEU:HG | 7 | 0.27 |
| (1,2) | 1:73:A:GLN:HE21 | 1:74:A:GLU:HG2 | 2 | 0.27 |
| (1,2) | 1:73:A:GLN:HE22 | 1:74:A:GLU:HG2 | 2 | 0.27 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 20 | 0.26 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 12 | 0.26 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 12 | 0.26 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 12 | 0.26 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 12 | 0.26 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 12 | 0.26 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 12 | 0.26 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 7 | 0.26 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 7 | 0.26 |
| (1,2189) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 1 | 0.26 |
| (1,2189) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 1 | 0.26 |
| (1,2189) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 1 | 0.26 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 9 | 0.26 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 7 | 0.26 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 7 | 0.26 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 7 | 0.26 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 7 | 0.26 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 7 | 0.26 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 7 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HA | 4 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HA | 4 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HA | 4 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HA | 4 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HA | 4 | 0.26 |
| (1,2031) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HA | 4 | 0.26 |
| (1,1963) | 1:49:A:LEU:HD11 | 1:201:A:CYS:HB2 | 6 | 0.26 |
| (1,1963) | 1:49:A:LEU:HD12 | 1:201:A:CYS:HB2 | 6 | 0.26 |
| (1,1963) | 1:49:A:LEU:HD13 | 1:201:A:CYS:HB2 | 6 | 0.26 |
| (1,1963) | 1:49:A:LEU:HD21 | 1:201:A:CYS:HB2 | 6 | 0.26 |
| (1,1963) | 1:49:A:LEU:HD22 | 1:201:A:CYS:HB2 | 6 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1963) | 1:49:A:LEU:HD23 | 1:201:A:CYS:HB2 | 6 | 0.26 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 1 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 16 | 0.26 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 16 | 0.26 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 6 | 0.26 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 6 | 0.26 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 6 | 0.26 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 14 | 0.26 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 14 | 0.26 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 14 | 0.26 |
| (1,1721) | 1:225:A:GLU:HG2 | 1:226:A:HIS:H | 3 | 0.26 |
| (1,1717) | 1:118:A:LEU:H | 1:120:A:GLU:HG2 | 15 | 0.26 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 9 | 0.26 |
| (1,1588) | 1:100:A:ALA:HB1 | 1:118:A:LEU:HG | 7 | 0.26 |
| (1,1588) | 1:100:A:ALA:HB2 | 1:118:A:LEU:HG | 7 | 0.26 |
| (1,1588) | 1:100:A:ALA:HB3 | 1:118:A:LEU:HG | 7 | 0.26 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 8 | 0.26 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 8 | 0.26 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 8 | 0.26 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 8 | 0.26 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 8 | 0.26 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 8 | 0.26 |
| (1,1493) | 1:207:A:ARG:HA | 1:207:A:ARG:HD2 | 3 | 0.26 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 14 | 0.26 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 7 | 0.26 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 7 | 0.26 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 7 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HG11 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HG12 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HG13 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HG11 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HG12 | 4 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1389) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HG13 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HG11 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HG12 | 4 | 0.26 |
| (1,1389) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HG13 | 4 | 0.26 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 8 | 0.26 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 8 | 0.26 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 8 | 0.26 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 7 | 0.26 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 7 | 0.26 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 7 | 0.26 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 15 | 0.26 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 15 | 0.26 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 15 | 0.26 |
| (1,1274) | 1:49:A:LEU:H | 1:164:A:LEU:HD11 | 8 | 0.26 |
| (1,1274) | 1:49:A:LEU:H | 1:164:A:LEU:HD12 | 8 | 0.26 |
| (1,1274) | 1:49:A:LEU:H | 1:164:A:LEU:HD13 | 8 | 0.26 |
| (1,1274) | 1:49:A:LEU:H | 1:164:A:LEU:HD21 | 8 | 0.26 |
| (1,1274) | 1:49:A:LEU:H | 1:164:A:LEU:HD22 | 8 | 0.26 |
| (1,1274) | 1:49:A:LEU:H | 1:164:A:LEU:HD23 | 8 | 0.26 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 8 | 0.26 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 8 | 0.26 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 16 | 0.26 |
| (1,1189) | 1:34:A:LEU:H | 1:38:A:SER:HB2 | 9 | 0.26 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 6 | 0.26 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 6 | 0.26 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 14 | 0.26 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 14 | 0.26 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 14 | 0.26 |
| (1,1036) | 1:98:A:ALA:H | 1:99:A:VAL:HA | 20 | 0.26 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 2 | 0.26 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG11 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG12 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG13 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG21 | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG22 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG23 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG11 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG12 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG13 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG21 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG22 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG23 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG11 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG12 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG13 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG21 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG22 | 10 | 0.26 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG23 | 10 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 4 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 9 | 0.26 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 9 | 0.26 |
| (1,844) | 1:132:A:CYS:HA | 1:135:A:LYS:HE2 | 14 | 0.26 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 15 | 0.26 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 15 | 0.26 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 15 | 0.26 |
| (1,787) | 1:28:A:PHE:HA | 1:217:A:VAL:HB | 6 | 0.26 |
| (1,759) | 1:148:A:GLN:H | 1:148:A:GLN:HG2 | 4 | 0.26 |
| (1,755) | 1:18:A:TYR:HD1 | 1:22:A:VAL:H | 10 | 0.26 |
| (1,755) | 1:18:A:TYR:HD2 | 1:22:A:VAL:H | 10 | 0.26 |
| (1,732) | 1:193:A:LEU:HG | 1:194:A:LEU:H | 14 | 0.26 |
| (1,669) | 1:189:A:SER:H | 1:193:A:LEU:H | 11 | 0.26 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 6 | 0.26 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 6 | 0.26 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 4 | 0.26 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 3 | 0.26 |
| (1,574) | 1:164:A:LEU:HG | 1:175:A:LEU:H | 3 | 0.26 |
| (1,528) | 1:60:A:GLU:HA | 1:63:A:ARG:H | 12 | 0.26 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 11 | 0.26 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 13 | 0.26 |
| (1,368) | 1:18:A:TYR:H | 1:19:A:ARG:HB2 | 6 | 0.26 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 18 | 0.26 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 19 | 0.26 |
| (1,254) | 1:209:A:GLN:HG2 | 1:210:A:GLY:H | 1 | 0.26 |
| (1,234) | 1:10:A:PRO:HA | 1:28:A:PHE:H | 13 | 0.26 |
| (1,234) | 1:10:A:PRO:HA | 1:28:A:PHE:H | 16 | 0.26 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 9 | 0.26 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 2 | 0.26 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 10 | 0.26 |
| (1,2370) | 1:221:A:LYS:HB2 | 1:222:A:ALA:HA | 13 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 6 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 6 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 6 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 6 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 6 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 6 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 15 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 15 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 15 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 15 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 15 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 15 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 16 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 16 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 16 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 16 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 16 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 16 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 7 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 7 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 7 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 7 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 7 | 0.25 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 7 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 10 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 10 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 10 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 10 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 10 | 0.25 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 10 | 0.25 |
| (1,2122) | 1:103:A:GLN:HB2 | 1:104:A:ASP:HB2 | 16 | 0.25 |
| (1,2074) | 1:81:A:PHE:HB2 | 1:96:A:ILE:HG21 | 3 | 0.25 |
| (1,2074) | 1:81:A:PHE:HB2 | 1:96:A:ILE:HG22 | 3 | 0.25 |
| (1,2074) | 1:81:A:PHE:HB2 | 1:96:A:ILE:HG23 | 3 | 0.25 |
| (1,2062) | 1:79:A:VAL:HG11 | 1:168:A:VAL:H | 5 | 0.25 |
| (1,2062) | 1:79:A:VAL:HG12 | 1:168:A:VAL:H | 5 | 0.25 |
| (1,2062) | 1:79:A:VAL:HG13 | 1:168:A:VAL:H | 5 | 0.25 |
| (1,2062) | 1:79:A:VAL:HG21 | 1:168:A:VAL:H | 5 | 0.25 |
| (1,2062) | 1:79:A:VAL:HG22 | 1:168:A:VAL:H | 5 | 0.25 |
| (1,2062) | 1:79:A:VAL:HG23 | 1:168:A:VAL:H | 5 | 0.25 |
| (1,2058) | 1:79:A:VAL:HG11 | 1:81:A:PHE:H | 4 | 0.25 |
| (1,2058) | 1:79:A:VAL:HG12 | 1:81:A:PHE:H | 4 | 0.25 |
| (1,2058) | 1:79:A:VAL:HG13 | 1:81:A:PHE:H | 4 | 0.25 |
| (1,2058) | 1:79:A:VAL:HG21 | 1:81:A:PHE:H | 4 | 0.25 |
| (1,2058) | 1:79:A:VAL:HG22 | 1:81:A:PHE:H | 4 | 0.25 |
| (1,2058) | 1:79:A:VAL:HG23 | 1:81:A:PHE:H | 4 | 0.25 |
| (1,2030) | 1:70:A:LEU:HD11 | 1:184:A:ASN:H | 10 | 0.25 |
| (1,2030) | 1:70:A:LEU:HD12 | 1:184:A:ASN:H | 10 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2030) | 1:70:A:LEU:HD13 | 1:184:A:ASN:H | 10 | 0.25 |
| (1,2030) | 1:70:A:LEU:HD21 | 1:184:A:ASN:H | 10 | 0.25 |
| (1,2030) | 1:70:A:LEU:HD22 | 1:184:A:ASN:H | 10 | 0.25 |
| (1,2030) | 1:70:A:LEU:HD23 | 1:184:A:ASN:H | 10 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD11 | 20 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD12 | 20 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD13 | 20 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD21 | 20 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD22 | 20 | 0.25 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD23 | 20 | 0.25 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 11 | 0.25 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD11 | 6 | 0.25 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD12 | 6 | 0.25 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD13 | 6 | 0.25 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD21 | 6 | 0.25 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD22 | 6 | 0.25 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD23 | 6 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD11 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD12 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD13 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD21 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD22 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD23 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD11 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD12 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD13 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD21 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD22 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD23 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD11 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD12 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD13 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD21 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD22 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD23 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD11 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD12 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD13 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD21 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD22 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD23 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD11 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD12 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD13 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD21 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD22 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD23 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD11 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD12 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD13 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD21 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD22 | 4 | 0.25 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD23 | 4 | 0.25 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 8 | 0.25 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE1 | 14 | 0.25 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE2 | 14 | 0.25 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE3 | 14 | 0.25 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 12 | 0.25 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 12 | 0.25 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 18 | 0.25 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 18 | 0.25 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 3 | 0.25 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 5 | 0.25 |
| (1,1763) | 1:19:A:ARG:HB2 | 1:20:A:LEU:HA | 12 | 0.25 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 4 | 0.25 |
| (1,1707) | 1:35:A:GLU:HG2 | 1:36:A:GLU:H | 20 | 0.25 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 7 | 0.25 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 7 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB1 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB2 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB3 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB1 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB2 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB3 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB1 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB2 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB3 | 13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB1 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB2 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB3 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB1 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB2 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB3 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB1 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB2 | 13 | 0.25 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB3 | 13 | 0.25 |
| (1,1576) | 1:175:A:LEU:HG | 1:183:A:VAL:H | 8 | 0.25 |
| (1,1572) | 1:221:A:LYS:HD2 | 1:222:A:ALA:H | 15 | 0.25 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 6 | 0.25 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 18 | 0.25 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 19 | 0.25 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 3 | 0.25 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 3 | 0.25 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 3 | 0.25 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB1 | 9 | 0.25 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB2 | 9 | 0.25 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB3 | 9 | 0.25 |
| (1,1500) | 1:130:A:ALA:HB1 | 1:132:A:CYS:H | 15 | 0.25 |
| (1,1500) | 1:130:A:ALA:HB2 | 1:132:A:CYS:H | 15 | 0.25 |
| (1,1500) | 1:130:A:ALA:HB3 | 1:132:A:CYS:H | 15 | 0.25 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 10 | 0.25 |
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 10 | 0.25 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 10 | 0.25 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 10 | 0.25 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 10 | 0.25 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 10 | 0.25 |
| (1,1411) | 1:136:A:ASN:HA | 1:140:A:GLN:HB2 | 10 | 0.25 |
| (1,1407) | 1:51:A:LEU:HD21 | 1:53:A:PHE:HB2 | 14 | 0.25 |
| (1,1407) | 1:51:A:LEU:HD22 | 1:53:A:PHE:HB2 | 14 | 0.25 |
| (1,1407) | 1:51:A:LEU:HD23 | 1:53:A:PHE:HB2 | 14 | 0.25 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 5 | 0.25 |
| (1,1350) | 1:156:A:ASP:HB2 | 1:158:A:VAL:HA | 14 | 0.25 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 7 | 0.25 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 9 | 0.25 |
| (1,1228) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HA | 3 | 0.25 |
| (1,1228) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HA | 3 | 0.25 |
| (1,1228) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HA | 3 | 0.25 |
| (1,1210) | 1:215:A:SER:HB2 | 1:216:A:ALA:H | 16 | 0.25 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE1 | 11 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE2 | 11 | 0.25 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE1 | 17 | 0.25 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE2 | 17 | 0.25 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 11 | 0.25 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 17 | 0.25 |
| (1,970) | 1:12:A:MET:HE1 | 1:151:A:GLN:H | 5 | 0.25 |
| (1,970) | 1:12:A:MET:HE2 | 1:151:A:GLN:H | 5 | 0.25 |
| (1,970) | 1:12:A:MET:HE3 | 1:151:A:GLN:H | 5 | 0.25 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 7 | 0.25 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 7 | 0.25 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 7 | 0.25 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 2 | 0.25 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 2 | 0.25 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 11 | 0.25 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 11 | 0.25 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 11 | 0.25 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 11 | 0.25 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 11 | 0.25 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 11 | 0.25 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 16 | 0.25 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 16 | 0.25 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 12 | 0.25 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD11 | 1 | 0.25 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD12 | 1 | 0.25 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD13 | 1 | 0.25 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD21 | 1 | 0.25 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD22 | 1 | 0.25 |
| (1,795) | 1:47:A:CYS:HA | 1:193:A:LEU:HD23 | 1 | 0.25 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 9 | 0.25 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 9 | 0.25 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 9 | 0.25 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 9 | 0.25 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD1 | 20 | 0.25 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD2 | 20 | 0.25 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 12 | 0.25 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 6 | 0.25 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 16 | 0.25 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 12 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 4 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 4 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 4 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 4 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 4 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 4 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 13 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 13 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 13 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 13 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 13 | 0.25 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 13 | 0.25 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 18 | 0.25 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 18 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,496) | 1:53:A:PHE:HB2 | 1:215:A:SER:H | 2 | 0.25 |
| (1,496) | 1:53:A:PHE:HB2 | 1:215:A:SER:H | 19 | 0.25 |
| (1,491) | 1:211:A:GLU:HA | 1:212:A:VAL:H | 8 | 0.25 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 6 | 0.25 |
| (1,403) | 1:99:A:VAL:HG11 | 1:103:A:GLN:HE21 | 15 | 0.25 |
| (1,403) | 1:99:A:VAL:HG12 | 1:103:A:GLN:HE21 | 15 | 0.25 |
| (1,403) | 1:99:A:VAL:HG13 | 1:103:A:GLN:HE21 | 15 | 0.25 |
| (1,403) | 1:99:A:VAL:HG21 | 1:103:A:GLN:HE21 | 15 | 0.25 |
| (1,403) | 1:99:A:VAL:HG22 | 1:103:A:GLN:HE21 | 15 | 0.25 |
| (1,403) | 1:99:A:VAL:HG23 | 1:103:A:GLN:HE21 | 15 | 0.25 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 9 | 0.25 |
| (1,358) | 1:127:A:GLU:H | 1:128:A:ASP:HB2 | 17 | 0.25 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 1 | 0.25 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 1 | 0.25 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 1 | 0.25 |
| (1,274) | 1:103:A:GLN:HE21 | 1:104:A:ASP:HB2 | 13 | 0.25 |
| (1,269) | 1:199:A:LYS:HE2 | 1:200:A:VAL:H | 19 | 0.25 |
| (1,224) | 1:167:A:ASN:HD21 | 1:190:A:GLU:HA | 4 | 0.25 |
| (1,179) | 1:213:A:ARG:H | 1:214:A:PHE:HB2 | 8 | 0.25 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 5 | 0.25 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 13 | 0.25 |
| (1,163) | 1:151:A:GLN:HB2 | 1:152:A:CYS:H | 10 | 0.25 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 7 | 0.25 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 8 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 8 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 8 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 8 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 8 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 8 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 19 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 19 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 19 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 19 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 19 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 19 | 0.24 |
| (1,2332) | 1:189:A:SER:HB2 | 1:193:A:LEU:HB2 | 1 | 0.24 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 1 | 0.24 |
| (1,2322) | 1:184:A:ASN:H | 1:184:A:ASN:HD21 | 3 | 0.24 |
| (1,2322) | 1:184:A:ASN:H | 1:184:A:ASN:HD22 | 3 | 0.24 |
| (1,2277) | 1:167:A:ASN:HD21 | 1:172:A:LEU:HB2 | 20 | 0.24 |
| (1,2277) | 1:167:A:ASN:HD22 | 1:172:A:LEU:HB2 | 20 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 3 | 0.24 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 3 | 0.24 |
| (1,2214) | 1:136:A:ASN:HD21 | 1:140:A:GLN:HB2 | 14 | 0.24 |
| (1,2214) | 1:136:A:ASN:HD22 | 1:140:A:GLN:HB2 | 14 | 0.24 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 11 | 0.24 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 12 | 0.24 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE21 | 2 | 0.24 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE22 | 2 | 0.24 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 20 | 0.24 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 20 | 0.24 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 20 | 0.24 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 11 | 0.24 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 11 | 0.24 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 11 | 0.24 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 11 | 0.24 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 11 | 0.24 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 11 | 0.24 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 3 | 0.24 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 3 | 0.24 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 4 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD11 | 1:198:A:ALA:HA | 12 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD12 | 1:198:A:ALA:HA | 12 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD13 | 1:198:A:ALA:HA | 12 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD21 | 1:198:A:ALA:HA | 12 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD22 | 1:198:A:ALA:HA | 12 | 0.24 |
| (1,1962) | 1:49:A:LEU:HD23 | 1:198:A:ALA:HA | 12 | 0.24 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 3 | 0.24 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 1 | 0.24 |
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 18 | 0.24 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 18 | 0.24 |
| (1,1844) | 1:12:A:MET:HE1 | 1:150:A:GLY:HA2 | 4 | 0.24 |
| (1,1844) | 1:12:A:MET:HE2 | 1:150:A:GLY:HA2 | 4 | 0.24 |
| (1,1844) | 1:12:A:MET:HE3 | 1:150:A:GLY:HA2 | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 17 | 0.24 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 17 | 0.24 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 17 | 0.24 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 10 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG21 | 18 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG22 | 18 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG23 | 18 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG21 | 18 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG22 | 18 | 0.24 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG23 | 18 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 8 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 8 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 8 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 10 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 10 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 10 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 13 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 13 | 0.24 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 13 | 0.24 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 3 | 0.24 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 13 | 0.24 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG11 | 6 | 0.24 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG12 | 6 | 0.24 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG13 | 6 | 0.24 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG21 | 6 | 0.24 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG22 | 6 | 0.24 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG23 | 6 | 0.24 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 17 | 0.24 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 17 | 0.24 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 17 | 0.24 |
| (1,1693) | 1:127:A:GLU:HG2 | 1:130:A:ALA:H | 12 | 0.24 |
| (1,1672) | 1:115:A:LYS:HB2 | 1:115:A:LYS:HE2 | 3 | 0.24 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 2 | 0.24 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 2 | 0.24 |
| (1,1658) | 1:158:A:VAL:HB | 1:159:A:ASN:H | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 7 | 0.24 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 19 | 0.24 |
| (1,1650) | 1:153:A:ARG:H | 1:153:A:ARG:HG2 | 1 | 0.24 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 8 | 0.24 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 19 | 0.24 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 20 | 0.24 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 20 | 0.24 |
| (1,1526) | 1:34:A:LEU:HD11 | 1:199:A:LYS:H | 18 | 0.24 |
| (1,1526) | 1:34:A:LEU:HD12 | 1:199:A:LYS:H | 18 | 0.24 |
| (1,1526) | 1:34:A:LEU:HD13 | 1:199:A:LYS:H | 18 | 0.24 |
| (1,1526) | 1:34:A:LEU:HD21 | 1:199:A:LYS:H | 18 | 0.24 |
| (1,1526) | 1:34:A:LEU:HD22 | 1:199:A:LYS:H | 18 | 0.24 |
| (1,1526) | 1:34:A:LEU:HD23 | 1:199:A:LYS:H | 18 | 0.24 |
| (1,1419) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HA | 12 | 0.24 |
| (1,1419) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HA | 12 | 0.24 |
| (1,1419) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HA | 12 | 0.24 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 3 | 0.24 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 16 | 0.24 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 15 | 0.24 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 15 | 0.24 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 15 | 0.24 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 20 | 0.24 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 13 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 5 | 0.24 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 5 | 0.24 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 1 | 0.24 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 9 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG11 | 11 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG12 | 11 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG13 | 11 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG21 | 11 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG22 | 11 | 0.24 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG23 | 11 | 0.24 |
| (1,1175) | 1:77:A:PRO:HA | 1:78:A:LYS:HD2 | 19 | 0.24 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 10 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 8 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 8 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 8 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 8 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 8 | 0.24 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 8 | 0.24 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 16 | 0.24 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 4 | 0.24 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 2 | 0.24 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 2 | 0.24 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 2 | 0.24 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 20 | 0.24 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 20 | 0.24 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 20 | 0.24 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 2 | 0.24 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 13 | 0.24 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 9 | 0.24 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 16 | 0.24 |
| (1,1014) | 1:122:A:GLU:HG2 | 1:123:A:LYS:HA | 17 | 0.24 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE1 | 20 | 0.24 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE2 | 20 | 0.24 |
| (1,967) | 1:120:A:GLU:HA | 1:124:A:MET:HE3 | 20 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 6 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 17 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 17 | 0.24 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 17 | 0.24 |
| (1,911) | 1:137:A:GLU:HA | 1:140:A:GLN:H | 18 | 0.24 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 9 | 0.24 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 9 | 0.24 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 9 | 0.24 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 9 | 0.24 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 9 | 0.24 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 9 | 0.24 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 15 | 0.24 |
| (1,787) | 1:28:A:PHE:HA | 1:217:A:VAL:HB | 2 | 0.24 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 10 | 0.24 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 16 | 0.24 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 15 | 0.24 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 19 | 0.24 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD1 | 6 | 0.24 |
| (1,593) | 1:130:A:ALA:H | 1:133:A:PHE:HD2 | 6 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 9 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 9 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 9 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 9 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 9 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 9 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 14 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 14 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 14 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 14 | 0.24 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 14 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 14 | 0.24 |
| (1,491) | 1:211:A:GLU:HA | 1:212:A:VAL:H | 19 | 0.24 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 10 | 0.24 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 16 | 0.24 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 8 | 0.24 |
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 8 | 0.24 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 8 | 0.24 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD1 | 11 | 0.24 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD2 | 11 | 0.24 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 13 | 0.24 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 13 | 0.24 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 13 | 0.24 |
| (1,305) | 1:31:A:VAL:H | 1:217:A:VAL:H | 19 | 0.24 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 13 | 0.24 |
| (1,190) | 1:193:A:LEU:HD11 | 1:194:A:LEU:H | 20 | 0.24 |
| (1,190) | 1:193:A:LEU:HD12 | 1:194:A:LEU:H | 20 | 0.24 |
| (1,190) | 1:193:A:LEU:HD13 | 1:194:A:LEU:H | 20 | 0.24 |
| (1,190) | 1:193:A:LEU:HD21 | 1:194:A:LEU:H | 20 | 0.24 |
| (1,190) | 1:193:A:LEU:HD22 | 1:194:A:LEU:H | 20 | 0.24 |
| (1,190) | 1:193:A:LEU:HD23 | 1:194:A:LEU:H | 20 | 0.24 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 14 | 0.24 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 2 | 0.24 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 2 | 0.24 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 2 | 0.24 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 18 | 0.24 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 2 | 0.24 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 17 | 0.23 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 17 | 0.23 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 17 | 0.23 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 17 | 0.23 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 17 | 0.23 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 17 | 0.23 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 7 | 0.23 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 13 | 0.23 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 13 | 0.23 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 13 | 0.23 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 2 | 0.23 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 2 | 0.23 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 2 | 0.23 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 2 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD11 | 1:166:A:ASN:HD21 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD11 | 1:166:A:ASN:HD22 | 14 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2251) | 1:164:A:LEU:HD12 | 1:166:A:ASN:HD21 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD12 | 1:166:A:ASN:HD22 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD13 | 1:166:A:ASN:HD21 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD13 | 1:166:A:ASN:HD22 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD21 | 1:166:A:ASN:HD21 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD21 | 1:166:A:ASN:HD22 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD22 | 1:166:A:ASN:HD21 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD22 | 1:166:A:ASN:HD22 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD23 | 1:166:A:ASN:HD21 | 14 | 0.23 |
| (1,2251) | 1:164:A:LEU:HD23 | 1:166:A:ASN:HD22 | 14 | 0.23 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE21 | 2 | 0.23 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE22 | 2 | 0.23 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG21 | 3 | 0.23 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG22 | 3 | 0.23 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG23 | 3 | 0.23 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 1 | 0.23 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD11 | 12 | 0.23 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD12 | 12 | 0.23 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD13 | 12 | 0.23 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD21 | 12 | 0.23 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD22 | 12 | 0.23 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD23 | 12 | 0.23 |
| (1,2125) | 1:103:A:GLN:HE22 | 1:122:A:GLU:HB2 | 9 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD21 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD22 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD21 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD22 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD21 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD22 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD21 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD22 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD21 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD22 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD21 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD22 | 3 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD21 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD22 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD21 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD22 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD21 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD22 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD21 | 12 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD22 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD21 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD22 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD21 | 12 | 0.23 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD22 | 12 | 0.23 |
| (1,2067) | 1:79:A:VAL:HG11 | 1:173:A:TYR:HA | 19 | 0.23 |
| (1,2067) | 1:79:A:VAL:HG12 | 1:173:A:TYR:HA | 19 | 0.23 |
| (1,2067) | 1:79:A:VAL:HG13 | 1:173:A:TYR:HA | 19 | 0.23 |
| (1,2067) | 1:79:A:VAL:HG21 | 1:173:A:TYR:HA | 19 | 0.23 |
| (1,2067) | 1:79:A:VAL:HG22 | 1:173:A:TYR:HA | 19 | 0.23 |
| (1,2067) | 1:79:A:VAL:HG23 | 1:173:A:TYR:HA | 19 | 0.23 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG11 | 12 | 0.23 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG12 | 12 | 0.23 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG13 | 12 | 0.23 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG21 | 12 | 0.23 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG22 | 12 | 0.23 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG23 | 12 | 0.23 |
| (1,2009) | 1:58:A:GLN:HB2 | 1:61:A:ASN:HD21 | 4 | 0.23 |
| (1,2009) | 1:58:A:GLN:HB2 | 1:61:A:ASN:HD22 | 4 | 0.23 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 18 | 0.23 |
| (1,1885) | 1:25:A:GLN:HE21 | 1:26:A:TRP:H | 6 | 0.23 |
| (1,1885) | 1:25:A:GLN:HE22 | 1:26:A:TRP:H | 6 | 0.23 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE1 | 16 | 0.23 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE2 | 16 | 0.23 |
| (1,1824) | 1:6:A:MET:HG2 | 1:12:A:MET:HE3 | 16 | 0.23 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG21 | 11 | 0.23 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG22 | 11 | 0.23 |
| (1,1784) | 1:80:A:TYR:HD1 | 1:121:A:THR:HG23 | 11 | 0.23 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG21 | 11 | 0.23 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG22 | 11 | 0.23 |
| (1,1784) | 1:80:A:TYR:HD2 | 1:121:A:THR:HG23 | 11 | 0.23 |
| (1,1763) | 1:19:A:ARG:HB2 | 1:20:A:LEU:HA | 4 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG11 | 14 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG12 | 14 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG13 | 14 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG21 | 14 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG22 | 14 | 0.23 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG23 | 14 | 0.23 |
| (1,1745) | 1:31:A:VAL:HB | 1:218:A:ALA:H | 8 | 0.23 |
| (1,1693) | 1:127:A:GLU:HG2 | 1:130:A:ALA:H | 16 | 0.23 |
| (1,1672) | 1:115:A:LYS:HB2 | 1:115:A:LYS:HE2 | 11 | 0.23 |
| (1,1650) | 1:153:A:ARG:H | 1:153:A:ARG:HG2 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 1 | 0.23 |
| (1,1572) | 1:221:A:LYS:HD2 | 1:222:A:ALA:H | 8 | 0.23 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 15 | 0.23 |
| (1,1528) | 1:91:A:GLY:HA2 | 1:93:A:ILE:HB | 13 | 0.23 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD1 | 14 | 0.23 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD2 | 14 | 0.23 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD1 | 14 | 0.23 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD2 | 14 | 0.23 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD1 | 14 | 0.23 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD2 | 14 | 0.23 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 20 | 0.23 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 20 | 0.23 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 20 | 0.23 |
| (1,1401) | 1:6:A:MET:HA | 1:7:A:GLU:HB2 | 12 | 0.23 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 14 | 0.23 |
| (1,1359) | 1:59:A:HIS:HA | 1:62:A:PHE:HD1 | 8 | 0.23 |
| (1,1359) | 1:59:A:HIS:HA | 1:62:A:PHE:HD2 | 8 | 0.23 |
| (1,1345) | 1:195:A:LYS:H | 1:195:A:LYS:HD2 | 5 | 0.23 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 13 | 0.23 |
| (1,1306) | 1:48:A:ALA:HB1 | 1:218:A:ALA:HA | 9 | 0.23 |
| (1,1306) | 1:48:A:ALA:HB2 | 1:218:A:ALA:HA | 9 | 0.23 |
| (1,1306) | 1:48:A:ALA:HB3 | 1:218:A:ALA:HA | 9 | 0.23 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 7 | 0.23 |
| (1,1257) | 1:58:A:GLN:HA | 1:61:A:ASN:HD22 | 15 | 0.23 |
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 7 | 0.23 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 5 | 0.23 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 5 | 0.23 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 11 | 0.23 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 11 | 0.23 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 19 | 0.23 |
| (1,1085) | 1:81:A:PHE:HE1 | 1:175:A:LEU:HB2 | 10 | 0.23 |
| (1,1085) | 1:81:A:PHE:HE2 | 1:175:A:LEU:HB2 | 10 | 0.23 |
| (1,1081) | 1:27:A:ARG:H | 1:28:A:PHE:HA | 2 | 0.23 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 17 | 0.23 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 4 | 0.23 |
| (1,1007) | 1:17:A:LEU:HA | 1:17:A:LEU:HG | 2 | 0.23 |
| (1,1007) | 1:17:A:LEU:HA | 1:17:A:LEU:HG | 7 | 0.23 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG11 | 13 | 0.23 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG12 | 13 | 0.23 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG13 | 13 | 0.23 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG21 | 13 | 0.23 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG22 | 13 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG23 | 13 | 0.23 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE1 | 5 | 0.23 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE2 | 5 | 0.23 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE3 | 5 | 0.23 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE1 | 16 | 0.23 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE2 | 16 | 0.23 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE3 | 16 | 0.23 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 9 | 0.23 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 1 | 0.23 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 1 | 0.23 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 1 | 0.23 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 5 | 0.23 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 5 | 0.23 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 5 | 0.23 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 12 | 0.23 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 20 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 20 | 0.23 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 20 | 0.23 |
| (1,910) | 1:39:A:LEU:HD11 | 1:195:A:LYS:HA | 1 | 0.23 |
| (1,910) | 1:39:A:LEU:HD12 | 1:195:A:LYS:HA | 1 | 0.23 |
| (1,910) | 1:39:A:LEU:HD13 | 1:195:A:LYS:HA | 1 | 0.23 |
| (1,910) | 1:39:A:LEU:HD11 | 1:195:A:LYS:HA | 14 | 0.23 |
| (1,910) | 1:39:A:LEU:HD12 | 1:195:A:LYS:HA | 14 | 0.23 |
| (1,910) | 1:39:A:LEU:HD13 | 1:195:A:LYS:HA | 14 | 0.23 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 11 | 0.23 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 3 | 0.23 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 3 | 0.23 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 3 | 0.23 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 8 | 0.23 |
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 8 | 0.23 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 8 | 0.23 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 8 | 0.23 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 8 | 0.23 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 8 | 0.23 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 17 | 0.23 |
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 17 | 0.23 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 17 | 0.23 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 17 | 0.23 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 17 | 0.23 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 17 | 0.23 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 8 | 0.23 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 18 | 0.23 |
| (1,665) | 1:187:A:ALA:HB1 | 1:188:A:SER:H | 18 | 0.23 |
| (1,665) | 1:187:A:ALA:HB2 | 1:188:A:SER:H | 18 | 0.23 |
| (1,665) | 1:187:A:ALA:HB3 | 1:188:A:SER:H | 18 | 0.23 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 17 | 0.23 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 17 | 0.23 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 17 | 0.23 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 8 | 0.23 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 16 | 0.23 |
| (1,496) | 1:53:A:PHE:HB2 | 1:215:A:SER:H | 7 | 0.23 |
| (1,403) | 1:99:A:VAL:HG11 | 1:103:A:GLN:HE21 | 19 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,403) | 1:99:A:VAL:HG12 | 1:103:A:GLN:HE21 | 19 | 0.23 |
| (1,403) | 1:99:A:VAL:HG13 | 1:103:A:GLN:HE21 | 19 | 0.23 |
| (1,403) | 1:99:A:VAL:HG21 | 1:103:A:GLN:HE21 | 19 | 0.23 |
| (1,403) | 1:99:A:VAL:HG22 | 1:103:A:GLN:HE21 | 19 | 0.23 |
| (1,403) | 1:99:A:VAL:HG23 | 1:103:A:GLN:HE21 | 19 | 0.23 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 14 | 0.23 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 14 | 0.23 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 14 | 0.23 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 19 | 0.23 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 19 | 0.23 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 19 | 0.23 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 6 | 0.23 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 2 | 0.23 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 2 | 0.23 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 2 | 0.23 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 5 | 0.23 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 5 | 0.23 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 5 | 0.23 |
| (1,250) | 1:123:A:LYS:H | 1:123:A:LYS:HG2 | 17 | 0.23 |
| (1,141) | 1:122:A:GLU:HA | 1:124:A:MET:H | 17 | 0.23 |
| (1,58) | 1:34:A:LEU:HB2 | 1:35:A:GLU:H | 1 | 0.23 |
| (1,30) | 1:23:A:ALA:H | 1:109:A:GLU:H | 1 | 0.23 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 3 | 0.22 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 3 | 0.22 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 3 | 0.22 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 3 | 0.22 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 3 | 0.22 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 3 | 0.22 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 10 | 0.22 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 10 | 0.22 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 10 | 0.22 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 4 | 0.22 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 4 | 0.22 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD21 | 7 | 0.22 |
| (1,2257) | 1:165:A:PHE:HD1 | 1:166:A:ASN:HD22 | 7 | 0.22 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD21 | 7 | 0.22 |
| (1,2257) | 1:165:A:PHE:HD2 | 1:166:A:ASN:HD22 | 7 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD11 | 1:166:A:ASN:HD21 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD11 | 1:166:A:ASN:HD22 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD12 | 1:166:A:ASN:HD21 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD12 | 1:166:A:ASN:HD22 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD13 | 1:166:A:ASN:HD21 | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2251) | 1:164:A:LEU:HD13 | 1:166:A:ASN:HD22 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD21 | 1:166:A:ASN:HD21 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD21 | 1:166:A:ASN:HD22 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD22 | 1:166:A:ASN:HD21 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD22 | 1:166:A:ASN:HD22 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD23 | 1:166:A:ASN:HD21 | 9 | 0.22 |
| (1,2251) | 1:164:A:LEU:HD23 | 1:166:A:ASN:HD22 | 9 | 0.22 |
| (1,2241) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HB2 | 1 | 0.22 |
| (1,2241) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HB2 | 1 | 0.22 |
| (1,2241) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HB2 | 1 | 0.22 |
| (1,2241) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HB2 | 1 | 0.22 |
| (1,2241) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HB2 | 1 | 0.22 |
| (1,2241) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HB2 | 1 | 0.22 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 4 | 0.22 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 4 | 0.22 |
| (1,2214) | 1:136:A:ASN:HD21 | 1:140:A:GLN:HB2 | 9 | 0.22 |
| (1,2214) | 1:136:A:ASN:HD22 | 1:140:A:GLN:HB2 | 9 | 0.22 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 2 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 6 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 15 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 15 | 0.22 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 15 | 0.22 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 16 | 0.22 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 1 | 0.22 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 1 | 0.22 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 1 | 0.22 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 1 | 0.22 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 1 | 0.22 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 1 | 0.22 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD11 | 15 | 0.22 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD12 | 15 | 0.22 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD13 | 15 | 0.22 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD21 | 15 | 0.22 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD22 | 15 | 0.22 |
| (1,2107) | 1:101:A:ASN:H | 1:106:A:LEU:HD23 | 15 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 17 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 17 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 17 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 17 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 17 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 17 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 20 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 20 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 20 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 20 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 20 | 0.22 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 20 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 11 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 11 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 11 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 11 | 0.22 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 11 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 11 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 20 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 20 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 20 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 20 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 20 | 0.22 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 20 | 0.22 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 11 | 0.22 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 12 | 0.22 |
| (1,1965) | 1:49:A:LEU:HD11 | 1:219:A:LEU:H | 8 | 0.22 |
| (1,1965) | 1:49:A:LEU:HD12 | 1:219:A:LEU:H | 8 | 0.22 |
| (1,1965) | 1:49:A:LEU:HD13 | 1:219:A:LEU:H | 8 | 0.22 |
| (1,1965) | 1:49:A:LEU:HD21 | 1:219:A:LEU:H | 8 | 0.22 |
| (1,1965) | 1:49:A:LEU:HD22 | 1:219:A:LEU:H | 8 | 0.22 |
| (1,1965) | 1:49:A:LEU:HD23 | 1:219:A:LEU:H | 8 | 0.22 |
| (1,1865) | 1:14:A:ASN:HD21 | 1:15:A:LYS:HE2 | 20 | 0.22 |
| (1,1865) | 1:14:A:ASN:HD22 | 1:15:A:LYS:HE2 | 20 | 0.22 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 1 | 0.22 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 1 | 0.22 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 1 | 0.22 |
| (1,1821) | 1:6:A:MET:HB2 | 1:147:A:ALA:HA | 6 | 0.22 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 15 | 0.22 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 15 | 0.22 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 15 | 0.22 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 15 | 0.22 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 15 | 0.22 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 15 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 3 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 3 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 3 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 5 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 5 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 5 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 6 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 6 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 6 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 15 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 15 | 0.22 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 15 | 0.22 |
| (1,1779) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HB2 | 15 | 0.22 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 14 | 0.22 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1732) | 1:122:A:GLU:HG2 | 1:123:A:LYS:HG2 | 12 | 0.22 |
| (1,1706) | 1:35:A:GLU:HA | 1:35:A:GLU:HG2 | 7 | 0.22 |
| (1,1675) | 1:25:A:GLN:HA | 1:221:A:LYS:HE2 | 5 | 0.22 |
| (1,1663) | 1:23:A:ALA:HA | 1:108:A:PHE:HB2 | 1 | 0.22 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 3 | 0.22 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 18 | 0.22 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 2 | 0.22 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 13 | 0.22 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 18 | 0.22 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 18 | 0.22 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 10 | 0.22 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 10 | 0.22 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 10 | 0.22 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 14 | 0.22 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 14 | 0.22 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 14 | 0.22 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 14 | 0.22 |
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 14 | 0.22 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 14 | 0.22 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 14 | 0.22 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 14 | 0.22 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 14 | 0.22 |
| (1,1466) | 1:19:A:ARG:HD2 | 1:145:A:ALA:H | 12 | 0.22 |
| (1,1417) | 1:77:A:PRO:HD2 | 1:78:A:LYS:HG2 | 18 | 0.22 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 6 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 9 | 0.22 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 9 | 0.22 |
| (1,1295) | 1:3:A:LEU:HG | 1:4:A:LYS:H | 18 | 0.22 |
| (1,1268) | 1:146:A:VAL:HG11 | 1:149:A:GLU:HG2 | 8 | 0.22 |
| (1,1268) | 1:146:A:VAL:HG12 | 1:149:A:GLU:HG2 | 8 | 0.22 |
| (1,1268) | 1:146:A:VAL:HG13 | 1:149:A:GLU:HG2 | 8 | 0.22 |
| (1,1268) | 1:146:A:VAL:HG21 | 1:149:A:GLU:HG2 | 8 | 0.22 |
| (1,1268) | 1:146:A:VAL:HG22 | 1:149:A:GLU:HG2 | 8 | 0.22 |
| (1,1268) | 1:146:A:VAL:HG23 | 1:149:A:GLU:HG2 | 8 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD11 | 11 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1245) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD12 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG21 | 1:52:A:LEU:HD13 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD11 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD12 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG22 | 1:52:A:LEU:HD13 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD11 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD12 | 11 | 0.22 |
| (1,1245) | 1:8:A:ILE:HG23 | 1:52:A:LEU:HD13 | 11 | 0.22 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 19 | 0.22 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 19 | 0.22 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 3 | 0.22 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 17 | 0.22 |
| (1,1157) | 1:28:A:PHE:HA | 1:217:A:VAL:HA | 4 | 0.22 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 18 | 0.22 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 18 | 0.22 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 18 | 0.22 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 18 | 0.22 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 18 | 0.22 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 18 | 0.22 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 3 | 0.22 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 19 | 0.22 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 6 | 0.22 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 6 | 0.22 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 6 | 0.22 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD11 | 2 | 0.22 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD12 | 2 | 0.22 |
| (1,1104) | 1:137:A:GLU:H | 1:139:A:ILE:HD13 | 2 | 0.22 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 20 | 0.22 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 20 | 0.22 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 20 | 0.22 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 15 | 0.22 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 15 | 0.22 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 15 | 0.22 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 2 | 0.22 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 8 | 0.22 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 8 | 0.22 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 8 | 0.22 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 19 | 0.22 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 5 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 5 | 0.22 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 5 | 0.22 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 3 | 0.22 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 8 | 0.22 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 3 | 0.22 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 14 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 14 | 0.22 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 14 | 0.22 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 4 | 0.22 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 4 | 0.22 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 4 | 0.22 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 4 | 0.22 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 4 | 0.22 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 4 | 0.22 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 19 | 0.22 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 19 | 0.22 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 19 | 0.22 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 19 | 0.22 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 19 | 0.22 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 19 | 0.22 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD11 | 11 | 0.22 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD12 | 11 | 0.22 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD13 | 11 | 0.22 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD21 | 11 | 0.22 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD22 | 11 | 0.22 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD23 | 11 | 0.22 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 4 | 0.22 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 12 | 0.22 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 12 | 0.22 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 12 | 0.22 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 12 | 0.22 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 12 | 0.22 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 12 | 0.22 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 1 | 0.22 |
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 1 | 0.22 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 1 | 0.22 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 8 | 0.22 |
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 8 | 0.22 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 8 | 0.22 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 19 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 19 | 0.22 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 19 | 0.22 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 4 | 0.22 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 11 | 0.22 |
| (1,787) | 1:28:A:PHE:HA | 1:217:A:VAL:HB | 14 | 0.22 |
| (1,759) | 1:148:A:GLN:H | 1:148:A:GLN:HG2 | 16 | 0.22 |
| (1,745) | 1:55:A:LEU:H | 1:160:A:PHE:HB2 | 15 | 0.22 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 14 | 0.22 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 2 | 0.22 |
| (1,664) | 1:172:A:LEU:H | 1:188:A:SER:H | 20 | 0.22 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 5 | 0.22 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 5 | 0.22 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 14 | 0.22 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 20 | 0.22 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 10 | 0.22 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 10 | 0.22 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 11 | 0.22 |
| (1,586) | 1:67:A:ILE:HD11 | 1:176:A:ASP:H | 3 | 0.22 |
| (1,586) | 1:67:A:ILE:HD12 | 1:176:A:ASP:H | 3 | 0.22 |
| (1,586) | 1:67:A:ILE:HD13 | 1:176:A:ASP:H | 3 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 1 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 1 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 1 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 1 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 1 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 1 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 7 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 7 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 7 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 7 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 7 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 7 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 19 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 19 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 19 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 19 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 19 | 0.22 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 19 | 0.22 |
| (1,518) | 1:3:A:LEU:H | 1:87:A:GLY:H | 18 | 0.22 |
| (1,416) | 1:193:A:LEU:HD11 | 1:197:A:ALA:H | 9 | 0.22 |
| (1,416) | 1:193:A:LEU:HD12 | 1:197:A:ALA:H | 9 | 0.22 |
| (1,416) | 1:193:A:LEU:HD13 | 1:197:A:ALA:H | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,416) | 1:193:A:LEU:HD21 | 1:197:A:ALA:H | 9 | 0.22 |
| (1,416) | 1:193:A:LEU:HD22 | 1:197:A:ALA:H | 9 | 0.22 |
| (1,416) | 1:193:A:LEU:HD23 | 1:197:A:ALA:H | 9 | 0.22 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 10 | 0.22 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 10 | 0.22 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 10 | 0.22 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 16 | 0.22 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 16 | 0.22 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 16 | 0.22 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 2 | 0.22 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 15 | 0.22 |
| (1,368) | 1:18:A:TYR:H | 1:19:A:ARG:HB2 | 11 | 0.22 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 3 | 0.22 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 15 | 0.22 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 6 | 0.22 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 11 | 0.22 |
| (1,163) | 1:151:A:GLN:HB2 | 1:152:A:CYS:H | 15 | 0.22 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD11 | 13 | 0.22 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD12 | 13 | 0.22 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD13 | 13 | 0.22 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD21 | 13 | 0.22 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD22 | 13 | 0.22 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD23 | 13 | 0.22 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 16 | 0.22 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 16 | 0.22 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 16 | 0.22 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 16 | 0.22 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 16 | 0.22 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 16 | 0.22 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 9 | 0.22 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 8 | 0.21 |
| (1,2345) | 1:200:A:VAL:HG11 | 1:203:A:GLU:HG2 | 6 | 0.21 |
| (1,2345) | 1:200:A:VAL:HG12 | 1:203:A:GLU:HG2 | 6 | 0.21 |
| (1,2345) | 1:200:A:VAL:HG13 | 1:203:A:GLU:HG2 | 6 | 0.21 |
| (1,2345) | 1:200:A:VAL:HG21 | 1:203:A:GLU:HG2 | 6 | 0.21 |
| (1,2345) | 1:200:A:VAL:HG22 | 1:203:A:GLU:HG2 | 6 | 0.21 |
| (1,2345) | 1:200:A:VAL:HG23 | 1:203:A:GLU:HG2 | 6 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 1 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 1 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 1 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 1 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 1 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 5 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 5 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 5 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 5 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 5 | 0.21 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 5 | 0.21 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 17 | 0.21 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 17 | 0.21 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 17 | 0.21 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 17 | 0.21 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 17 | 0.21 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 17 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 11 | 0.21 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 11 | 0.21 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 13 | 0.21 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 19 | 0.21 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 19 | 0.21 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 19 | 0.21 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 19 | 0.21 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 19 | 0.21 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 19 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HB | 3 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HB | 3 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HB | 3 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG21 | 1:168:A:VAL:HB | 3 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG22 | 1:168:A:VAL:HB | 3 | 0.21 |
| (1,2063) | 1:79:A:VAL:HG23 | 1:168:A:VAL:HB | 3 | 0.21 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 1 | 0.21 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 1 | 0.21 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 1 | 0.21 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 1 | 0.21 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 1 | 0.21 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE21 | 13 | 0.21 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE22 | 13 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD1 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD2 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD1 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD2 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD1 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD2 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD1 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD2 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD1 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD2 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD1 | 6 | 0.21 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD2 | 6 | 0.21 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 4 | 0.21 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 14 | 0.21 |
| (1,1885) | 1:25:A:GLN:HE21 | 1:26:A:TRP:H | 12 | 0.21 |
| (1,1885) | 1:25:A:GLN:HE22 | 1:26:A:TRP:H | 12 | 0.21 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD11 | 6 | 0.21 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD12 | 6 | 0.21 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD13 | 6 | 0.21 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD21 | 6 | 0.21 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD22 | 6 | 0.21 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD23 | 6 | 0.21 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 19 | 0.21 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 19 | 0.21 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 19 | 0.21 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 19 | 0.21 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 19 | 0.21 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 19 | 0.21 |
| (1,1805) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HB | 12 | 0.21 |
| (1,1805) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HB | 12 | 0.21 |
| (1,1805) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HB | 12 | 0.21 |
| (1,1805) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HB | 12 | 0.21 |
| (1,1805) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HB | 12 | 0.21 |
| (1,1805) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HB | 12 | 0.21 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 6 | 0.21 |
| (1,1718) | 1:210:A:GLY:H | 1:211:A:GLU:HG2 | 13 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 3 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 3 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 7 | 0.21 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 7 | 0.21 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 18 | 0.21 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 10 | 0.21 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 10 | 0.21 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 11 | 0.21 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 10 | 0.21 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 10 | 0.21 |
| (1,1576) | 1:175:A:LEU:HG | 1:183:A:VAL:H | 4 | 0.21 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB1 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB2 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG11 | 1:142:A:ALA:HB3 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB1 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB2 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG12 | 1:142:A:ALA:HB3 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB1 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB2 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG13 | 1:142:A:ALA:HB3 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB1 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB2 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG21 | 1:142:A:ALA:HB3 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB1 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB2 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG22 | 1:142:A:ALA:HB3 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB1 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB2 | 7 | 0.21 |
| (1,1513) | 1:16:A:VAL:HG23 | 1:142:A:ALA:HB3 | 7 | 0.21 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 6 | 0.21 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 6 | 0.21 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 6 | 0.21 |
| (1,1476) | 1:153:A:ARG:H | 1:153:A:ARG:HD2 | 6 | 0.21 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 1 | 0.21 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 1 | 0.21 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 1 | 0.21 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD21 | 11 | 0.21 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD22 | 11 | 0.21 |
| (1,1343) | 1:26:A:TRP:HE1 | 1:106:A:LEU:HD23 | 11 | 0.21 |
| (1,1322) | 1:64:A:LYS:HA | 1:64:A:LYS:HE2 | 15 | 0.21 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE1 | 8 | 0.21 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE2 | 8 | 0.21 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 6 | 0.21 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 4 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 18 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 18 | 0.21 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 18 | 0.21 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 7 | 0.21 |
| (1,1210) | 1:215:A:SER:HB2 | 1:216:A:ALA:H | 5 | 0.21 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE1 | 1 | 0.21 |
| (1,1178) | 1:75:A:VAL:HA | 1:81:A:PHE:HE2 | 1 | 0.21 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 5 | 0.21 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 5 | 0.21 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 5 | 0.21 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 20 | 0.21 |
| (1,1121) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HG2 | 3 | 0.21 |
| (1,1121) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HG2 | 3 | 0.21 |
| (1,1121) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HG2 | 3 | 0.21 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD11 | 12 | 0.21 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD12 | 12 | 0.21 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD13 | 12 | 0.21 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD11 | 12 | 0.21 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD12 | 12 | 0.21 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD13 | 12 | 0.21 |
| (1,1085) | 1:81:A:PHE:HE1 | 1:175:A:LEU:HB2 | 12 | 0.21 |
| (1,1085) | 1:81:A:PHE:HE2 | 1:175:A:LEU:HB2 | 12 | 0.21 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 17 | 0.21 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 17 | 0.21 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 17 | 0.21 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 10 | 0.21 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 10 | 0.21 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 14 | 0.21 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 20 | 0.21 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 20 | 0.21 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 20 | 0.21 |
| (1,1007) | 1:17:A:LEU:HA | 1:17:A:LEU:HG | 10 | 0.21 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG11 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG12 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG13 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG21 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG22 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG23 | 19 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG11 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG12 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG13 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG21 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG22 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG23 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG11 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG12 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG13 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG21 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG22 | 19 | 0.21 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG23 | 19 | 0.21 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 15 | 0.21 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 15 | 0.21 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 10 | 0.21 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 10 | 0.21 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 10 | 0.21 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 10 | 0.21 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 10 | 0.21 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 10 | 0.21 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 19 | 0.21 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 19 | 0.21 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 14 | 0.21 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 14 | 0.21 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 14 | 0.21 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 14 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 14 | 0.21 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 14 | 0.21 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 2 | 0.21 |
| (1,859) | 1:155:A:ASP:H | 1:155:A:ASP:HB2 | 1 | 0.21 |
| (1,812) | 1:93:A:ILE:HG21 | 1:165:A:PHE:H | 6 | 0.21 |
| (1,812) | 1:93:A:ILE:HG22 | 1:165:A:PHE:H | 6 | 0.21 |
| (1,812) | 1:93:A:ILE:HG23 | 1:165:A:PHE:H | 6 | 0.21 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 20 | 0.21 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 20 | 0.21 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 20 | 0.21 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 5 | 0.21 |
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 5 | 0.21 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 5 | 0.21 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 5 | 0.21 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 5 | 0.21 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 5 | 0.21 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 19 | 0.21 |
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 19 | 0.21 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 19 | 0.21 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 19 | 0.21 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 19 | 0.21 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 19 | 0.21 |
| (1,714) | 1:18:A:TYR:H | 1:18:A:TYR:HE1 | 9 | 0.21 |
| (1,714) | 1:18:A:TYR:H | 1:18:A:TYR:HE2 | 9 | 0.21 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 16 | 0.21 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 18 | 0.21 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 15 | 0.21 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 8 | 0.21 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 8 | 0.21 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 8 | 0.21 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 14 | 0.21 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 14 | 0.21 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 14 | 0.21 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 5 | 0.21 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 13 | 0.21 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 6 | 0.21 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 6 | 0.21 |
| (1,454) | 1:112:A:SER:H | 1:115:A:LYS:HB2 | 16 | 0.21 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 2 | 0.21 |
| (1,432) | 1:80:A:TYR:HE1 | 1:124:A:MET:H | 13 | 0.21 |
| (1,377) | 1:31:A:VAL:HG11 | 1:32:A:LEU:H | 8 | 0.21 |
| (1,377) | 1:31:A:VAL:HG12 | 1:32:A:LEU:H | 8 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,377) | 1:31:A:VAL:HG13 | 1:32:A:LEU:H | 8 | 0.21 |
| (1,377) | 1:31:A:VAL:HG21 | 1:32:A:LEU:H | 8 | 0.21 |
| (1,377) | 1:31:A:VAL:HG22 | 1:32:A:LEU:H | 8 | 0.21 |
| (1,377) | 1:31:A:VAL:HG23 | 1:32:A:LEU:H | 8 | 0.21 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 17 | 0.21 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 5 | 0.21 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 14 | 0.21 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 15 | 0.21 |
| (1,358) | 1:127:A:GLU:H | 1:128:A:ASP:HB2 | 4 | 0.21 |
| (1,358) | 1:127:A:GLU:H | 1:128:A:ASP:HB2 | 12 | 0.21 |
| (1,350) | 1:208:A:GLU:HG2 | 1:209:A:GLN:H | 20 | 0.21 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD1 | 19 | 0.21 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD2 | 19 | 0.21 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 12 | 0.21 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 18 | 0.21 |
| (1,234) | 1:10:A:PRO:HA | 1:28:A:PHE:H | 10 | 0.21 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 8 | 0.21 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 13 | 0.21 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 13 | 0.21 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 13 | 0.21 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 16 | 0.21 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 16 | 0.21 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 16 | 0.21 |
| (1,39) | 1:27:A:ARG:H | 1:221:A:LYS:HA | 1 | 0.21 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG11 | 15 | 0.2 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG12 | 15 | 0.2 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG13 | 15 | 0.2 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG21 | 15 | 0.2 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG22 | 15 | 0.2 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG23 | 15 | 0.2 |
| (1,2320) | 1:183:A:VAL:HG11 | 1:185:A:HIS:HA | 15 | 0.2 |
| (1,2320) | 1:183:A:VAL:HG12 | 1:185:A:HIS:HA | 15 | 0.2 |
| (1,2320) | 1:183:A:VAL:HG13 | 1:185:A:HIS:HA | 15 | 0.2 |
| (1,2320) | 1:183:A:VAL:HG21 | 1:185:A:HIS:HA | 15 | 0.2 |
| (1,2320) | 1:183:A:VAL:HG22 | 1:185:A:HIS:HA | 15 | 0.2 |
| (1,2320) | 1:183:A:VAL:HG23 | 1:185:A:HIS:HA | 15 | 0.2 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 1 | 0.2 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 1 | 0.2 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 1 | 0.2 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 1 | 0.2 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 1 | 0.2 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 1 | 0.2 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 1 | 0.2 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 1 | 0.2 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 1 | 0.2 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 1 | 0.2 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 1 | 0.2 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 20 | 0.2 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 20 | 0.2 |
| (1,2181) | 1:122:A:GLU:HB2 | 1:123:A:LYS:H | 5 | 0.2 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD11 | 17 | 0.2 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD12 | 17 | 0.2 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD13 | 17 | 0.2 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD21 | 17 | 0.2 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD22 | 17 | 0.2 |
| (1,2168) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HD23 | 17 | 0.2 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE21 | 12 | 0.2 |
| (1,2080) | 1:86:A:ILE:H | 1:140:A:GLN:HE22 | 12 | 0.2 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 16 | 0.2 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 16 | 0.2 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 16 | 0.2 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 17 | 0.2 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 17 | 0.2 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 17 | 0.2 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE21 | 11 | 0.2 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE22 | 11 | 0.2 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 2 | 0.2 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 2 | 0.2 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 2 | 0.2 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 2 | 0.2 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 2 | 0.2 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 2 | 0.2 |
| (1,2007) | 1:58:A:GLN:HB2 | 1:59:A:HIS:H | 18 | 0.2 |
| (1,1997) | 1:55:A:LEU:HD11 | 1:161:A:HIS:H | 16 | 0.2 |
| (1,1997) | 1:55:A:LEU:HD12 | 1:161:A:HIS:H | 16 | 0.2 |
| (1,1997) | 1:55:A:LEU:HD13 | 1:161:A:HIS:H | 16 | 0.2 |
| (1,1997) | 1:55:A:LEU:HD21 | 1:161:A:HIS:H | 16 | 0.2 |
| (1,1997) | 1:55:A:LEU:HD22 | 1:161:A:HIS:H | 16 | 0.2 |
| (1,1997) | 1:55:A:LEU:HD23 | 1:161:A:HIS:H | 16 | 0.2 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 7 | 0.2 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 17 | 0.2 |
| (1,1874) | 1:17:A:LEU:HD11 | 1:95:A:LEU:HB2 | 14 | 0.2 |
| (1,1874) | 1:17:A:LEU:HD12 | 1:95:A:LEU:HB2 | 14 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1874) | 1:17:A:LEU:HD13 | 1:95:A:LEU:HB2 | 14 | 0.2 |
| (1,1874) | 1:17:A:LEU:HD21 | 1:95:A:LEU:HB2 | 14 | 0.2 |
| (1,1874) | 1:17:A:LEU:HD22 | 1:95:A:LEU:HB2 | 14 | 0.2 |
| (1,1874) | 1:17:A:LEU:HD23 | 1:95:A:LEU:HB2 | 14 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD11 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD12 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD13 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD21 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD22 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD23 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD11 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD12 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD13 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD21 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD22 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD23 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD11 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD12 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD13 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD21 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD22 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD23 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD11 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD12 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD13 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD21 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD22 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD23 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD11 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD12 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD13 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD21 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD22 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD23 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD11 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD12 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD13 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD21 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD22 | 8 | 0.2 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD23 | 8 | 0.2 |
| (1,1817) | 1:4:A:LYS:H | 1:144:A:ASP:HB2 | 9 | 0.2 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG11 | 8 | 0.2 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG12 | 8 | 0.2 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG13 | 8 | 0.2 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG21 | 8 | 0.2 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG22 | 8 | 0.2 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG23 | 8 | 0.2 |
| (1,1724) | 1:74:A:GLU:HG2 | 1:75:A:VAL:H | 6 | 0.2 |
| (1,1717) | 1:118:A:LEU:H | 1:120:A:GLU:HG2 | 19 | 0.2 |
| (1,1707) | 1:35:A:GLU:HG2 | 1:36:A:GLU:H | 3 | 0.2 |
| (1,1689) | 1:14:A:ASN:HB2 | 1:15:A:LYS:HE2 | 7 | 0.2 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 20 | 0.2 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG11 | 10 | 0.2 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG12 | 10 | 0.2 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG13 | 10 | 0.2 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG21 | 10 | 0.2 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG22 | 10 | 0.2 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG23 | 10 | 0.2 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 16 | 0.2 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 16 | 0.2 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 16 | 0.2 |
| (1,1577) | 1:164:A:LEU:HD11 | 1:175:A:LEU:HG | 1 | 0.2 |
| (1,1577) | 1:164:A:LEU:HD12 | 1:175:A:LEU:HG | 1 | 0.2 |
| (1,1577) | 1:164:A:LEU:HD13 | 1:175:A:LEU:HG | 1 | 0.2 |
| (1,1577) | 1:164:A:LEU:HD21 | 1:175:A:LEU:HG | 1 | 0.2 |
| (1,1577) | 1:164:A:LEU:HD22 | 1:175:A:LEU:HG | 1 | 0.2 |
| (1,1577) | 1:164:A:LEU:HD23 | 1:175:A:LEU:HG | 1 | 0.2 |
| (1,1572) | 1:221:A:LYS:HD2 | 1:222:A:ALA:H | 17 | 0.2 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB1 | 12 | 0.2 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB2 | 12 | 0.2 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB3 | 12 | 0.2 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD1 | 6 | 0.2 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD2 | 6 | 0.2 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD1 | 6 | 0.2 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD2 | 6 | 0.2 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD1 | 6 | 0.2 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD2 | 6 | 0.2 |
| (1,1398) | 1:81:A:PHE:H | 1:82:A:MET:HA | 6 | 0.2 |
| (1,1356) | 1:117:A:PHE:HA | 1:119:A:SER:H | 7 | 0.2 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 12 | 0.2 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 10 | 0.2 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 2 | 0.2 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 10 | 0.2 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 7 | 0.2 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 8 | 0.2 |
| (1,1284) | 1:80:A:TYR:HD1 | 1:100:A:ALA:HA | 9 | 0.2 |
| (1,1284) | 1:80:A:TYR:HD2 | 1:100:A:ALA:HA | 9 | 0.2 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 5 | 0.2 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 17 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 3 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 12 | 0.2 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 12 | 0.2 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 17 | 0.2 |
| (1,1203) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HD1 | 1 | 0.2 |
| (1,1203) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HD2 | 1 | 0.2 |
| (1,1203) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HD1 | 1 | 0.2 |
| (1,1203) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HD2 | 1 | 0.2 |
| (1,1203) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HD1 | 1 | 0.2 |
| (1,1203) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HD2 | 1 | 0.2 |
| (1,1202) | 1:79:A:VAL:H | 1:168:A:VAL:HG21 | 7 | 0.2 |
| (1,1202) | 1:79:A:VAL:H | 1:168:A:VAL:HG22 | 7 | 0.2 |
| (1,1202) | 1:79:A:VAL:H | 1:168:A:VAL:HG23 | 7 | 0.2 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 2 | 0.2 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 5 | 0.2 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD1 | 1 | 0.2 |
| (1,1149) | 1:52:A:LEU:HA | 1:214:A:PHE:HD2 | 1 | 0.2 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 5 | 0.2 |
| (1,1085) | 1:81:A:PHE:HE1 | 1:175:A:LEU:HB2 | 14 | 0.2 |
| (1,1085) | 1:81:A:PHE:HE2 | 1:175:A:LEU:HB2 | 14 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 4 | 0.2 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 4 | 0.2 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 4 | 0.2 |
| (1,1058) | 1:12:A:MET:HA | 1:15:A:LYS:HE2 | 12 | 0.2 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 10 | 0.2 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 12 | 0.2 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 15 | 0.2 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 10 | 0.2 |
| (1,844) | 1:132:A:CYS:HA | 1:135:A:LYS:HE2 | 10 | 0.2 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 19 | 0.2 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 19 | 0.2 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 19 | 0.2 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB1 | 5 | 0.2 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB2 | 5 | 0.2 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB3 | 5 | 0.2 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG21 | 11 | 0.2 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG22 | 11 | 0.2 |
| (1,810) | 1:93:A:ILE:HA | 1:96:A:ILE:HG23 | 11 | 0.2 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 17 | 0.2 |
| (1,744) | 1:146:A:VAL:HG11 | 1:150:A:GLY:H | 7 | 0.2 |
| (1,744) | 1:146:A:VAL:HG12 | 1:150:A:GLY:H | 7 | 0.2 |
| (1,744) | 1:146:A:VAL:HG13 | 1:150:A:GLY:H | 7 | 0.2 |
| (1,744) | 1:146:A:VAL:HG21 | 1:150:A:GLY:H | 7 | 0.2 |
| (1,744) | 1:146:A:VAL:HG22 | 1:150:A:GLY:H | 7 | 0.2 |
| (1,744) | 1:146:A:VAL:HG23 | 1:150:A:GLY:H | 7 | 0.2 |
| (1,731) | 1:194:A:LEU:H | 1:196:A:ASP:H | 5 | 0.2 |
| (1,706) | 1:73:A:GLN:HA | 1:74:A:GLU:H | 12 | 0.2 |
| (1,684) | 1:168:A:VAL:HA | 1:171:A:HIS:H | 11 | 0.2 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 20 | 0.2 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 20 | 0.2 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 11 | 0.2 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 20 | 0.2 |
| (1,543) | 1:60:A:GLU:H | 1:62:A:PHE:H | 8 | 0.2 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 7 | 0.2 |
| (1,496) | 1:53:A:PHE:HB2 | 1:215:A:SER:H | 9 | 0.2 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 3 | 0.2 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 3 | 0.2 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 3 | 0.2 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 3 | 0.2 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 12 | 0.2 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 12 | 0.2 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 12 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,377) | 1:31:A:VAL:HG11 | 1:32:A:LEU:H | 18 | 0.2 |
| (1,377) | 1:31:A:VAL:HG12 | 1:32:A:LEU:H | 18 | 0.2 |
| (1,377) | 1:31:A:VAL:HG13 | 1:32:A:LEU:H | 18 | 0.2 |
| (1,377) | 1:31:A:VAL:HG21 | 1:32:A:LEU:H | 18 | 0.2 |
| (1,377) | 1:31:A:VAL:HG22 | 1:32:A:LEU:H | 18 | 0.2 |
| (1,377) | 1:31:A:VAL:HG23 | 1:32:A:LEU:H | 18 | 0.2 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD1 | 1 | 0.2 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD2 | 1 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 6 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 6 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 6 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 8 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 8 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 8 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 16 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 16 | 0.2 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 16 | 0.2 |
| (1,305) | 1:31:A:VAL:H | 1:217:A:VAL:H | 17 | 0.2 |
| (1,246) | 1:164:A:LEU:HD11 | 1:175:A:LEU:H | 5 | 0.2 |
| (1,246) | 1:164:A:LEU:HD12 | 1:175:A:LEU:H | 5 | 0.2 |
| (1,246) | 1:164:A:LEU:HD13 | 1:175:A:LEU:H | 5 | 0.2 |
| (1,246) | 1:164:A:LEU:HD21 | 1:175:A:LEU:H | 5 | 0.2 |
| (1,246) | 1:164:A:LEU:HD22 | 1:175:A:LEU:H | 5 | 0.2 |
| (1,246) | 1:164:A:LEU:HD23 | 1:175:A:LEU:H | 5 | 0.2 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 11 | 0.2 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 15 | 0.2 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 16 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 11 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 11 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 11 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 18 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 18 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 18 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 19 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 19 | 0.2 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 19 | 0.2 |
| (1,2362) | 1:219:A:LEU:HD11 | 1:222:A:ALA:H | 2 | 0.19 |
| (1,2362) | 1:219:A:LEU:HD12 | 1:222:A:ALA:H | 2 | 0.19 |
| (1,2362) | 1:219:A:LEU:HD13 | 1:222:A:ALA:H | 2 | 0.19 |
| (1,2362) | 1:219:A:LEU:HD21 | 1:222:A:ALA:H | 2 | 0.19 |
| (1,2362) | 1:219:A:LEU:HD22 | 1:222:A:ALA:H | 2 | 0.19 |
| (1,2362) | 1:219:A:LEU:HD23 | 1:222:A:ALA:H | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2326) | 1:189:A:SER:HB2 | 1:190:A:GLU:HB2 | 11 | 0.19 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 16 | 0.19 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 16 | 0.19 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 16 | 0.19 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 16 | 0.19 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 16 | 0.19 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 16 | 0.19 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 8 | 0.19 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 8 | 0.19 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 8 | 0.19 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 8 | 0.19 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 8 | 0.19 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 8 | 0.19 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 5 | 0.19 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 5 | 0.19 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 10 | 0.19 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 10 | 0.19 |
| (1,2192) | 1:129:A:ARG:HG2 | 1:132:A:CYS:HB2 | 18 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 3 | 0.19 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 3 | 0.19 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 1 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 18 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 18 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 18 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 18 | 0.19 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 18 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 18 | 0.19 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 19 | 0.19 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 19 | 0.19 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 19 | 0.19 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 19 | 0.19 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 19 | 0.19 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 19 | 0.19 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 5 | 0.19 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 5 | 0.19 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 16 | 0.19 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 16 | 0.19 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 12 | 0.19 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 10 | 0.19 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD11 | 8 | 0.19 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD12 | 8 | 0.19 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD13 | 8 | 0.19 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD21 | 8 | 0.19 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD22 | 8 | 0.19 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD23 | 8 | 0.19 |
| (1,1933) | 1:36:A:GLU:HG2 | 1:40:A:GLY:H | 7 | 0.19 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 18 | 0.19 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 11 | 0.19 |
| (1,1873) | 1:17:A:LEU:HD11 | 1:95:A:LEU:HA | 14 | 0.19 |
| (1,1873) | 1:17:A:LEU:HD12 | 1:95:A:LEU:HA | 14 | 0.19 |
| (1,1873) | 1:17:A:LEU:HD13 | 1:95:A:LEU:HA | 14 | 0.19 |
| (1,1873) | 1:17:A:LEU:HD21 | 1:95:A:LEU:HA | 14 | 0.19 |
| (1,1873) | 1:17:A:LEU:HD22 | 1:95:A:LEU:HA | 14 | 0.19 |
| (1,1873) | 1:17:A:LEU:HD23 | 1:95:A:LEU:HA | 14 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 3 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 3 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 3 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 3 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 3 | 0.19 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 3 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 1 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 1 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 1 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 16 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 16 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 16 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 17 | 0.19 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 17 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 17 | 0.19 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 1 | 0.19 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 20 | 0.19 |
| (1,1769) | 1:56:A:THR:HA | 1:60:A:GLU:HB2 | 8 | 0.19 |
| (1,1730) | 1:108:A:PHE:HA | 1:109:A:GLU:HG2 | 7 | 0.19 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 1 | 0.19 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 1 | 0.19 |
| (1,1575) | 1:175:A:LEU:HG | 1:176:A:ASP:H | 6 | 0.19 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 17 | 0.19 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB1 | 3 | 0.19 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB2 | 3 | 0.19 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB3 | 3 | 0.19 |
| (1,1500) | 1:130:A:ALA:HB1 | 1:132:A:CYS:H | 9 | 0.19 |
| (1,1500) | 1:130:A:ALA:HB2 | 1:132:A:CYS:H | 9 | 0.19 |
| (1,1500) | 1:130:A:ALA:HB3 | 1:132:A:CYS:H | 9 | 0.19 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 3 | 0.19 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 19 | 0.19 |
| (1,1428) | 1:23:A:ALA:HB1 | 1:107:A:GLY:HA2 | 1 | 0.19 |
| (1,1428) | 1:23:A:ALA:HB2 | 1:107:A:GLY:HA2 | 1 | 0.19 |
| (1,1428) | 1:23:A:ALA:HB3 | 1:107:A:GLY:HA2 | 1 | 0.19 |
| (1,1401) | 1:6:A:MET:HA | 1:7:A:GLU:HB2 | 10 | 0.19 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 17 | 0.19 |
| (1,1310) | 1:67:A:ILE:HB | 1:181:A:PHE:HA | 8 | 0.19 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 12 | 0.19 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 13 | 0.19 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 5 | 0.19 |
| (1,1257) | 1:58:A:GLN:HA | 1:61:A:ASN:HD22 | 4 | 0.19 |
| (1,1199) | 1:5:A:PRO:HA | 1:88:A:ASN:H | 13 | 0.19 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 5 | 0.19 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 4 | 0.19 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 4 | 0.19 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 4 | 0.19 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 4 | 0.19 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 4 | 0.19 |
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 4 | 0.19 |
| (1,1117) | 1:197:A:ALA:HA | 1:201:A:CYS:HB2 | 16 | 0.19 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 1 | 0.19 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 1 | 0.19 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 1 | 0.19 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 3 | 0.19 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 3 | 0.19 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 3 | 0.19 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 9 | 0.19 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 17 | 0.19 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 17 | 0.19 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 17 | 0.19 |
| (1,1038) | 1:99:A:VAL:HA | 1:103:A:GLN:HG2 | 6 | 0.19 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD21 | 12 | 0.19 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD22 | 12 | 0.19 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD23 | 12 | 0.19 |
| (1,962) | 1:124:A:MET:HE1 | 1:129:A:ARG:H | 12 | 0.19 |
| (1,962) | 1:124:A:MET:HE2 | 1:129:A:ARG:H | 12 | 0.19 |
| (1,962) | 1:124:A:MET:HE3 | 1:129:A:ARG:H | 12 | 0.19 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 17 | 0.19 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 17 | 0.19 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 11 | 0.19 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD21 | 13 | 0.19 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD22 | 13 | 0.19 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD23 | 13 | 0.19 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 13 | 0.19 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 13 | 0.19 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 13 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 13 | 0.19 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 19 | 0.19 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 19 | 0.19 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 12 | 0.19 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 12 | 0.19 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 12 | 0.19 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 12 | 0.19 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 12 | 0.19 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 12 | 0.19 |
| (1,919) | 1:48:A:ALA:HA | 1:193:A:LEU:HD11 | 13 | 0.19 |
| (1,919) | 1:48:A:ALA:HA | 1:193:A:LEU:HD12 | 13 | 0.19 |
| (1,919) | 1:48:A:ALA:HA | 1:193:A:LEU:HD13 | 13 | 0.19 |
| (1,919) | 1:48:A:ALA:HA | 1:193:A:LEU:HD21 | 13 | 0.19 |
| (1,919) | 1:48:A:ALA:HA | 1:193:A:LEU:HD22 | 13 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,919) | 1:48:A:ALA:HA | 1:193:A:LEU:HD23 | 13 | 0.19 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD11 | 20 | 0.19 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD12 | 20 | 0.19 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD13 | 20 | 0.19 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD21 | 20 | 0.19 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD22 | 20 | 0.19 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD23 | 20 | 0.19 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 3 | 0.19 |
| (1,844) | 1:132:A:CYS:HA | 1:135:A:LYS:HE2 | 2 | 0.19 |
| (1,844) | 1:132:A:CYS:HA | 1:135:A:LYS:HE2 | 17 | 0.19 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 1 | 0.19 |
| (1,787) | 1:28:A:PHE:HA | 1:217:A:VAL:HB | 8 | 0.19 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 20 | 0.19 |
| (1,704) | 1:23:A:ALA:HA | 1:25:A:GLN:H | 9 | 0.19 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 9 | 0.19 |
| (1,684) | 1:168:A:VAL:HA | 1:171:A:HIS:H | 13 | 0.19 |
| (1,681) | 1:194:A:LEU:HA | 1:197:A:ALA:H | 16 | 0.19 |
| (1,667) | 1:189:A:SER:H | 1:192:A:THR:H | 7 | 0.19 |
| (1,665) | 1:187:A:ALA:HB1 | 1:188:A:SER:H | 11 | 0.19 |
| (1,665) | 1:187:A:ALA:HB2 | 1:188:A:SER:H | 11 | 0.19 |
| (1,665) | 1:187:A:ALA:HB3 | 1:188:A:SER:H | 11 | 0.19 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 11 | 0.19 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 11 | 0.19 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 11 | 0.19 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 17 | 0.19 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 8 | 0.19 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 8 | 0.19 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 8 | 0.19 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 8 | 0.19 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 8 | 0.19 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 8 | 0.19 |
| (1,535) | 1:117:A:PHE:HA | 1:120:A:GLU:H | 12 | 0.19 |
| (1,535) | 1:117:A:PHE:HA | 1:120:A:GLU:H | 17 | 0.19 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 3 | 0.19 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 13 | 0.19 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 17 | 0.19 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 14 | 0.19 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 14 | 0.19 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 20 | 0.19 |
| (1,269) | 1:199:A:LYS:HE2 | 1:200:A:VAL:H | 3 | 0.19 |
| (1,246) | 1:164:A:LEU:HD11 | 1:175:A:LEU:H | 1 | 0.19 |
| (1,246) | 1:164:A:LEU:HD12 | 1:175:A:LEU:H | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,246) | 1:164:A:LEU:HD13 | 1:175:A:LEU:H | 1 | 0.19 |
| (1,246) | 1:164:A:LEU:HD21 | 1:175:A:LEU:H | 1 | 0.19 |
| (1,246) | 1:164:A:LEU:HD22 | 1:175:A:LEU:H | 1 | 0.19 |
| (1,246) | 1:164:A:LEU:HD23 | 1:175:A:LEU:H | 1 | 0.19 |
| (1,246) | 1:164:A:LEU:HD11 | 1:175:A:LEU:H | 7 | 0.19 |
| (1,246) | 1:164:A:LEU:HD12 | 1:175:A:LEU:H | 7 | 0.19 |
| (1,246) | 1:164:A:LEU:HD13 | 1:175:A:LEU:H | 7 | 0.19 |
| (1,246) | 1:164:A:LEU:HD21 | 1:175:A:LEU:H | 7 | 0.19 |
| (1,246) | 1:164:A:LEU:HD22 | 1:175:A:LEU:H | 7 | 0.19 |
| (1,246) | 1:164:A:LEU:HD23 | 1:175:A:LEU:H | 7 | 0.19 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 3 | 0.19 |
| (1,141) | 1:122:A:GLU:HA | 1:124:A:MET:H | 14 | 0.19 |
| (1,141) | 1:122:A:GLU:HA | 1:124:A:MET:H | 16 | 0.19 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 8 | 0.19 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 8 | 0.19 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 8 | 0.19 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 8 | 0.19 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 8 | 0.19 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 8 | 0.19 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 6 | 0.18 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 9 | 0.18 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 12 | 0.18 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 12 | 0.18 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 12 | 0.18 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 12 | 0.18 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 12 | 0.18 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 12 | 0.18 |
| (1,2277) | 1:167:A:ASN:HD21 | 1:172:A:LEU:HB2 | 12 | 0.18 |
| (1,2277) | 1:167:A:ASN:HD22 | 1:172:A:LEU:HB2 | 12 | 0.18 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 5 | 0.18 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 5 | 0.18 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 5 | 0.18 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 5 | 0.18 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 5 | 0.18 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 5 | 0.18 |
| (1,2232) | 1:151:A:GLN:HB2 | 1:151:A:GLN:HE21 | 19 | 0.18 |
| (1,2232) | 1:151:A:GLN:HB2 | 1:151:A:GLN:HE22 | 19 | 0.18 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG21 | 20 | 0.18 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG22 | 20 | 0.18 |
| (1,2205) | 1:136:A:ASN:HB2 | 1:139:A:ILE:HG23 | 20 | 0.18 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 5 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG21 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG22 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG11 | 1:139:A:ILE:HG23 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG21 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG22 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG12 | 1:139:A:ILE:HG23 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG21 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG22 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG13 | 1:139:A:ILE:HG23 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG21 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG22 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG21 | 1:139:A:ILE:HG23 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG21 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG22 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG22 | 1:139:A:ILE:HG23 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG21 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG22 | 17 | 0.18 |
| (1,2154) | 1:113:A:VAL:HG23 | 1:139:A:ILE:HG23 | 17 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 8 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 8 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 8 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 8 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 8 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 8 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 12 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 12 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 12 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 12 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 12 | 0.18 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 12 | 0.18 |
| (1,2031) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HA | 14 | 0.18 |
| (1,2031) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HA | 14 | 0.18 |
| (1,2031) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HA | 14 | 0.18 |
| (1,2031) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HA | 14 | 0.18 |
| (1,2031) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HA | 14 | 0.18 |
| (1,2031) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HA | 14 | 0.18 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 16 | 0.18 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 16 | 0.18 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 16 | 0.18 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 16 | 0.18 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 16 | 0.18 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 16 | 0.18 |
| (1,2007) | 1:58:A:GLN:HB2 | 1:59:A:HIS:H | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2007) | 1:58:A:GLN:HB2 | 1:59:A:HIS:H | 11 | 0.18 |
| (1,1962) | 1:49:A:LEU:HD11 | 1:198:A:ALA:HA | 14 | 0.18 |
| (1,1962) | 1:49:A:LEU:HD12 | 1:198:A:ALA:HA | 14 | 0.18 |
| (1,1962) | 1:49:A:LEU:HD13 | 1:198:A:ALA:HA | 14 | 0.18 |
| (1,1962) | 1:49:A:LEU:HD21 | 1:198:A:ALA:HA | 14 | 0.18 |
| (1,1962) | 1:49:A:LEU:HD22 | 1:198:A:ALA:HA | 14 | 0.18 |
| (1,1962) | 1:49:A:LEU:HD23 | 1:198:A:ALA:HA | 14 | 0.18 |
| (1,1961) | 1:49:A:LEU:HD11 | 1:198:A:ALA:H | 20 | 0.18 |
| (1,1961) | 1:49:A:LEU:HD12 | 1:198:A:ALA:H | 20 | 0.18 |
| (1,1961) | 1:49:A:LEU:HD13 | 1:198:A:ALA:H | 20 | 0.18 |
| (1,1961) | 1:49:A:LEU:HD21 | 1:198:A:ALA:H | 20 | 0.18 |
| (1,1961) | 1:49:A:LEU:HD22 | 1:198:A:ALA:H | 20 | 0.18 |
| (1,1961) | 1:49:A:LEU:HD23 | 1:198:A:ALA:H | 20 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD1 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD11 | 1:165:A:PHE:HD2 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD1 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD12 | 1:165:A:PHE:HD2 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD1 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD13 | 1:165:A:PHE:HD2 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD1 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD21 | 1:165:A:PHE:HD2 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD1 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD22 | 1:165:A:PHE:HD2 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD1 | 7 | 0.18 |
| (1,1959) | 1:49:A:LEU:HD23 | 1:165:A:PHE:HD2 | 7 | 0.18 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 15 | 0.18 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 15 | 0.18 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 8 | 0.18 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 8 | 0.18 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 8 | 0.18 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 8 | 0.18 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 8 | 0.18 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 8 | 0.18 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 8 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD11 | 1 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD12 | 1 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD13 | 1 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD21 | 1 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD22 | 1 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD23 | 1 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD11 | 7 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD12 | 7 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD13 | 7 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD21 | 7 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD22 | 7 | 0.18 |
| (1,1872) | 1:17:A:LEU:HB2 | 1:95:A:LEU:HD23 | 7 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD1 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD11 | 1:28:A:PHE:HD2 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD1 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD12 | 1:28:A:PHE:HD2 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD1 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD13 | 1:28:A:PHE:HD2 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD1 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD21 | 1:28:A:PHE:HD2 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD1 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD22 | 1:28:A:PHE:HD2 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD1 | 5 | 0.18 |
| (1,1855) | 1:13:A:LEU:HD23 | 1:28:A:PHE:HD2 | 5 | 0.18 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE1 | 12 | 0.18 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE2 | 12 | 0.18 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE3 | 12 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 2 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 2 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 2 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 2 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 2 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 2 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 17 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 17 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 17 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 17 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 17 | 0.18 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 17 | 0.18 |
| (1,1807) | 1:3:A:LEU:HD11 | 1:89:A:SER:HB2 | 4 | 0.18 |
| (1,1807) | 1:3:A:LEU:HD12 | 1:89:A:SER:HB2 | 4 | 0.18 |
| (1,1807) | 1:3:A:LEU:HD13 | 1:89:A:SER:HB2 | 4 | 0.18 |
| (1,1807) | 1:3:A:LEU:HD21 | 1:89:A:SER:HB2 | 4 | 0.18 |
| (1,1807) | 1:3:A:LEU:HD22 | 1:89:A:SER:HB2 | 4 | 0.18 |
| (1,1807) | 1:3:A:LEU:HD23 | 1:89:A:SER:HB2 | 4 | 0.18 |
| (1,1805) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HB | 7 | 0.18 |
| (1,1805) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HB | 7 | 0.18 |
| (1,1805) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HB | 7 | 0.18 |
| (1,1805) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HB | 7 | 0.18 |
| (1,1805) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HB | 7 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1805) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HB | 7 | 0.18 |
| (1,1788) | 1:14:A:ASN:HB2 | 1:18:A:TYR:HE1 | 19 | 0.18 |
| (1,1788) | 1:14:A:ASN:HB2 | 1:18:A:TYR:HE2 | 19 | 0.18 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE1 | 18 | 0.18 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE2 | 18 | 0.18 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 18 | 0.18 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 18 | 0.18 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 18 | 0.18 |
| (1,1763) | 1:19:A:ARG:HB2 | 1:20:A:LEU:HA | 3 | 0.18 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG11 | 13 | 0.18 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG12 | 13 | 0.18 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG13 | 13 | 0.18 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG21 | 13 | 0.18 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG22 | 13 | 0.18 |
| (1,1760) | 1:153:A:ARG:HB2 | 1:154:A:VAL:HG23 | 13 | 0.18 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 1 | 0.18 |
| (1,1707) | 1:35:A:GLU:HG2 | 1:36:A:GLU:H | 1 | 0.18 |
| (1,1707) | 1:35:A:GLU:HG2 | 1:36:A:GLU:H | 18 | 0.18 |
| (1,1693) | 1:127:A:GLU:HG2 | 1:130:A:ALA:H | 15 | 0.18 |
| (1,1676) | 1:25:A:GLN:HG2 | 1:221:A:LYS:HE2 | 15 | 0.18 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 14 | 0.18 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 15 | 0.18 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 17 | 0.18 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 17 | 0.18 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 17 | 0.18 |
| (1,1568) | 1:221:A:LYS:HA | 1:222:A:ALA:HB1 | 17 | 0.18 |
| (1,1568) | 1:221:A:LYS:HA | 1:222:A:ALA:HB2 | 17 | 0.18 |
| (1,1568) | 1:221:A:LYS:HA | 1:222:A:ALA:HB3 | 17 | 0.18 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 18 | 0.18 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 4 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD11 | 1:198:A:ALA:HB1 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD11 | 1:198:A:ALA:HB2 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD11 | 1:198:A:ALA:HB3 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD12 | 1:198:A:ALA:HB1 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD12 | 1:198:A:ALA:HB2 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD12 | 1:198:A:ALA:HB3 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD13 | 1:198:A:ALA:HB1 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD13 | 1:198:A:ALA:HB2 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD13 | 1:198:A:ALA:HB3 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD21 | 1:198:A:ALA:HB1 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD21 | 1:198:A:ALA:HB2 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD21 | 1:198:A:ALA:HB3 | 14 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1514) | 1:34:A:LEU:HD22 | 1:198:A:ALA:HB1 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD22 | 1:198:A:ALA:HB2 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD22 | 1:198:A:ALA:HB3 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD23 | 1:198:A:ALA:HB1 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD23 | 1:198:A:ALA:HB2 | 14 | 0.18 |
| (1,1514) | 1:34:A:LEU:HD23 | 1:198:A:ALA:HB3 | 14 | 0.18 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 16 | 0.18 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 12 | 0.18 |
| (1,1356) | 1:117:A:PHE:HA | 1:119:A:SER:H | 17 | 0.18 |
| (1,1345) | 1:195:A:LYS:H | 1:195:A:LYS:HD2 | 12 | 0.18 |
| (1,1328) | 1:80:A:TYR:HA | 1:80:A:TYR:HE2 | 14 | 0.18 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE1 | 11 | 0.18 |
| (1,1315) | 1:75:A:VAL:HB | 1:81:A:PHE:HE2 | 11 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 19 | 0.18 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 19 | 0.18 |
| (1,1233) | 1:154:A:VAL:HA | 1:156:A:ASP:HB2 | 1 | 0.18 |
| (1,1233) | 1:154:A:VAL:HA | 1:156:A:ASP:HB2 | 10 | 0.18 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG11 | 20 | 0.18 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG12 | 20 | 0.18 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG13 | 20 | 0.18 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG21 | 20 | 0.18 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG22 | 20 | 0.18 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG23 | 20 | 0.18 |
| (1,1176) | 1:75:A:VAL:HG11 | 1:77:A:PRO:HA | 3 | 0.18 |
| (1,1176) | 1:75:A:VAL:HG12 | 1:77:A:PRO:HA | 3 | 0.18 |
| (1,1176) | 1:75:A:VAL:HG13 | 1:77:A:PRO:HA | 3 | 0.18 |
| (1,1176) | 1:75:A:VAL:HG21 | 1:77:A:PRO:HA | 3 | 0.18 |
| (1,1176) | 1:75:A:VAL:HG22 | 1:77:A:PRO:HA | 3 | 0.18 |
| (1,1176) | 1:75:A:VAL:HG23 | 1:77:A:PRO:HA | 3 | 0.18 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 15 | 0.18 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 15 | 0.18 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 15 | 0.18 |
| (1,1157) | 1:28:A:PHE:HA | 1:217:A:VAL:HA | 11 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG21 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG22 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1119) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HG23 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG21 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG22 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HG23 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG21 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG22 | 17 | 0.18 |
| (1,1119) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HG23 | 17 | 0.18 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 1 | 0.18 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD11 | 7 | 0.18 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD12 | 7 | 0.18 |
| (1,1105) | 1:133:A:PHE:HD1 | 1:139:A:ILE:HD13 | 7 | 0.18 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD11 | 7 | 0.18 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD12 | 7 | 0.18 |
| (1,1105) | 1:133:A:PHE:HD2 | 1:139:A:ILE:HD13 | 7 | 0.18 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG21 | 4 | 0.18 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG22 | 4 | 0.18 |
| (1,1071) | 1:201:A:CYS:HB2 | 1:205:A:THR:HG23 | 4 | 0.18 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 1 | 0.18 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 1 | 0.18 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 1 | 0.18 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 5 | 0.18 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 5 | 0.18 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 5 | 0.18 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG11 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG12 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG13 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG21 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG22 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG23 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG11 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG12 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG13 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG21 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG22 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG23 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG11 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG12 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG13 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG21 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG22 | 7 | 0.18 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG23 | 7 | 0.18 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 9 | 0.18 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 9 | 0.18 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 12 | 0.18 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 10 | 0.18 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 10 | 0.18 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 10 | 0.18 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 14 | 0.18 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 14 | 0.18 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 14 | 0.18 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 4 | 0.18 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 4 | 0.18 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 5 | 0.18 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 5 | 0.18 |
| (1,901) | 1:188:A:SER:HB2 | 1:193:A:LEU:HG | 1 | 0.18 |
| (1,859) | 1:155:A:ASP:H | 1:155:A:ASP:HB2 | 16 | 0.18 |
| (1,765) | 1:192:A:THR:HA | 1:194:A:LEU:H | 10 | 0.18 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 1 | 0.18 |
| (1,727) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE22 | 5 | 0.18 |
| (1,727) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE22 | 5 | 0.18 |
| (1,727) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE22 | 5 | 0.18 |
| (1,726) | 1:99:A:VAL:HB | 1:100:A:ALA:H | 3 | 0.18 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD1 | 9 | 0.18 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD2 | 9 | 0.18 |
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 17 | 0.18 |
| (1,681) | 1:194:A:LEU:HA | 1:197:A:ALA:H | 1 | 0.18 |
| (1,669) | 1:189:A:SER:H | 1:193:A:LEU:H | 15 | 0.18 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 9 | 0.18 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 9 | 0.18 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 12 | 0.18 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 2 | 0.18 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 4 | 0.18 |
| (1,616) | 1:4:A:LYS:H | 1:144:A:ASP:HA | 9 | 0.18 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 5 | 0.18 |
| (1,543) | 1:60:A:GLU:H | 1:62:A:PHE:H | 11 | 0.18 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 2 | 0.18 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 10 | 0.18 |
| (1,512) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 7 | 0.18 |
| (1,458) | 1:156:A:ASP:HA | 1:158:A:VAL:H | 8 | 0.18 |
| (1,439) | 1:133:A:PHE:H | 1:135:A:LYS:HG2 | 20 | 0.18 |
| (1,377) | 1:31:A:VAL:HG11 | 1:32:A:LEU:H | 17 | 0.18 |
| (1,377) | 1:31:A:VAL:HG12 | 1:32:A:LEU:H | 17 | 0.18 |
| (1,377) | 1:31:A:VAL:HG13 | 1:32:A:LEU:H | 17 | 0.18 |
| (1,377) | 1:31:A:VAL:HG21 | 1:32:A:LEU:H | 17 | 0.18 |
| (1,377) | 1:31:A:VAL:HG22 | 1:32:A:LEU:H | 17 | 0.18 |
| (1,377) | 1:31:A:VAL:HG23 | 1:32:A:LEU:H | 17 | 0.18 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 19 | 0.18 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD1 | 4 | 0.18 |
| (1,345) | 1:214:A:PHE:H | 1:214:A:PHE:HD2 | 4 | 0.18 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 8 | 0.18 |
| (1,317) | 1:206:A:GLU:H | 1:208:A:GLU:H | 20 | 0.18 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 3 | 0.18 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 3 | 0.18 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 3 | 0.18 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 14 | 0.18 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 16 | 0.18 |
| (1,72) | 1:48:A:ALA:H | 1:218:A:ALA:HA | 9 | 0.18 |
| (1,39) | 1:27:A:ARG:H | 1:221:A:LYS:HA | 5 | 0.18 |
| (1,2362) | 1:219:A:LEU:HD11 | 1:222:A:ALA:H | 13 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD12 | 1:222:A:ALA:H | 13 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD13 | 1:222:A:ALA:H | 13 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD21 | 1:222:A:ALA:H | 13 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD22 | 1:222:A:ALA:H | 13 | 0.17 |
| (1,2362) | 1:219:A:LEU:HD23 | 1:222:A:ALA:H | 13 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB1 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB2 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD11 | 1:197:A:ALA:HB3 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB1 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB2 | 12 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2303) | 1:172:A:LEU:HD12 | 1:197:A:ALA:HB3 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB1 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB2 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD13 | 1:197:A:ALA:HB3 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB1 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB2 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HB3 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB1 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB2 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HB3 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB1 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB2 | 12 | 0.17 |
| (1,2303) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HB3 | 12 | 0.17 |
| (1,2277) | 1:167:A:ASN:HD21 | 1:172:A:LEU:HB2 | 19 | 0.17 |
| (1,2277) | 1:167:A:ASN:HD22 | 1:172:A:LEU:HB2 | 19 | 0.17 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 14 | 0.17 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 14 | 0.17 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE21 | 17 | 0.17 |
| (1,2231) | 1:151:A:GLN:HA | 1:151:A:GLN:HE22 | 17 | 0.17 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 14 | 0.17 |
| (1,2189) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 5 | 0.17 |
| (1,2189) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 5 | 0.17 |
| (1,2189) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 5 | 0.17 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 18 | 0.17 |
| (1,2085) | 1:86:A:ILE:HD11 | 1:140:A:GLN:HE21 | 19 | 0.17 |
| (1,2085) | 1:86:A:ILE:HD11 | 1:140:A:GLN:HE22 | 19 | 0.17 |
| (1,2085) | 1:86:A:ILE:HD12 | 1:140:A:GLN:HE21 | 19 | 0.17 |
| (1,2085) | 1:86:A:ILE:HD12 | 1:140:A:GLN:HE22 | 19 | 0.17 |
| (1,2085) | 1:86:A:ILE:HD13 | 1:140:A:GLN:HE21 | 19 | 0.17 |
| (1,2085) | 1:86:A:ILE:HD13 | 1:140:A:GLN:HE22 | 19 | 0.17 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE21 | 20 | 0.17 |
| (1,2082) | 1:86:A:ILE:HB | 1:140:A:GLN:HE22 | 20 | 0.17 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 8 | 0.17 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 8 | 0.17 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 8 | 0.17 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG11 | 16 | 0.17 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG12 | 16 | 0.17 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG13 | 16 | 0.17 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG21 | 16 | 0.17 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG22 | 16 | 0.17 |
| (1,2054) | 1:79:A:VAL:H | 1:168:A:VAL:HG23 | 16 | 0.17 |
| (1,2018) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HD2 | 14 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 14 | 0.17 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 14 | 0.17 |
| (1,1922) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HB2 | 18 | 0.17 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 12 | 0.17 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 10 | 0.17 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 7 | 0.17 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 7 | 0.17 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 7 | 0.17 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 7 | 0.17 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 7 | 0.17 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 7 | 0.17 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 18 | 0.17 |
| (1,1848) | 1:13:A:LEU:HA | 1:17:A:LEU:HB2 | 5 | 0.17 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 20 | 0.17 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 20 | 0.17 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 20 | 0.17 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 20 | 0.17 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 20 | 0.17 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 20 | 0.17 |
| (1,1814) | 1:3:A:LEU:HD11 | 1:143:A:HIS:H | 9 | 0.17 |
| (1,1814) | 1:3:A:LEU:HD12 | 1:143:A:HIS:H | 9 | 0.17 |
| (1,1814) | 1:3:A:LEU:HD13 | 1:143:A:HIS:H | 9 | 0.17 |
| (1,1814) | 1:3:A:LEU:HD21 | 1:143:A:HIS:H | 9 | 0.17 |
| (1,1814) | 1:3:A:LEU:HD22 | 1:143:A:HIS:H | 9 | 0.17 |
| (1,1814) | 1:3:A:LEU:HD23 | 1:143:A:HIS:H | 9 | 0.17 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 14 | 0.17 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 14 | 0.17 |
| (1,1793) | 1:18:A:TYR:HD1 | 1:21:A:GLY:HA2 | 3 | 0.17 |
| (1,1793) | 1:18:A:TYR:HD2 | 1:21:A:GLY:HA2 | 3 | 0.17 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD1 | 7 | 0.17 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD2 | 7 | 0.17 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 7 | 0.17 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 7 | 0.17 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 7 | 0.17 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 11 | 0.17 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 11 | 0.17 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 11 | 0.17 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 14 | 0.17 |
| (1,1759) | 1:152:A:CYS:HB2 | 1:153:A:ARG:HB2 | 6 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 18 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 18 | 0.17 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 18 | 0.17 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 14 | 0.17 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 14 | 0.17 |
| (1,1668) | 1:96:A:ILE:HD11 | 1:117:A:PHE:HD1 | 16 | 0.17 |
| (1,1668) | 1:96:A:ILE:HD11 | 1:117:A:PHE:HD2 | 16 | 0.17 |
| (1,1668) | 1:96:A:ILE:HD12 | 1:117:A:PHE:HD1 | 16 | 0.17 |
| (1,1668) | 1:96:A:ILE:HD12 | 1:117:A:PHE:HD2 | 16 | 0.17 |
| (1,1668) | 1:96:A:ILE:HD13 | 1:117:A:PHE:HD1 | 16 | 0.17 |
| (1,1668) | 1:96:A:ILE:HD13 | 1:117:A:PHE:HD2 | 16 | 0.17 |
| (1,1663) | 1:23:A:ALA:HA | 1:108:A:PHE:HB2 | 17 | 0.17 |
| (1,1653) | 1:113:A:VAL:H | 1:114:A:LEU:HG | 13 | 0.17 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 14 | 0.17 |
| (1,1639) | 1:19:A:ARG:H | 1:20:A:LEU:HB2 | 9 | 0.17 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 15 | 0.17 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 15 | 0.17 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 15 | 0.17 |
| (1,1577) | 1:164:A:LEU:HD11 | 1:175:A:LEU:HG | 7 | 0.17 |
| (1,1577) | 1:164:A:LEU:HD12 | 1:175:A:LEU:HG | 7 | 0.17 |
| (1,1577) | 1:164:A:LEU:HD13 | 1:175:A:LEU:HG | 7 | 0.17 |
| (1,1577) | 1:164:A:LEU:HD21 | 1:175:A:LEU:HG | 7 | 0.17 |
| (1,1577) | 1:164:A:LEU:HD22 | 1:175:A:LEU:HG | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1577) | 1:164:A:LEU:HD23 | 1:175:A:LEU:HG | 7 | 0.17 |
| (1,1576) | 1:175:A:LEU:HG | 1:183:A:VAL:H | 6 | 0.17 |
| (1,1564) | 1:74:A:GLU:HA | 1:75:A:VAL:H | 8 | 0.17 |
| (1,1564) | 1:74:A:GLU:HA | 1:75:A:VAL:H | 18 | 0.17 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 6 | 0.17 |
| (1,1541) | 1:112:A:SER:HA | 1:113:A:VAL:HB | 18 | 0.17 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD1 | 2 | 0.17 |
| (1,1501) | 1:130:A:ALA:HB1 | 1:133:A:PHE:HD2 | 2 | 0.17 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD1 | 2 | 0.17 |
| (1,1501) | 1:130:A:ALA:HB2 | 1:133:A:PHE:HD2 | 2 | 0.17 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD1 | 2 | 0.17 |
| (1,1501) | 1:130:A:ALA:HB3 | 1:133:A:PHE:HD2 | 2 | 0.17 |
| (1,1479) | 1:50:A:LEU:HB2 | 1:217:A:VAL:H | 3 | 0.17 |
| (1,1475) | 1:212:A:VAL:HG11 | 1:213:A:ARG:HD2 | 5 | 0.17 |
| (1,1475) | 1:212:A:VAL:HG12 | 1:213:A:ARG:HD2 | 5 | 0.17 |
| (1,1475) | 1:212:A:VAL:HG13 | 1:213:A:ARG:HD2 | 5 | 0.17 |
| (1,1475) | 1:212:A:VAL:HG21 | 1:213:A:ARG:HD2 | 5 | 0.17 |
| (1,1475) | 1:212:A:VAL:HG22 | 1:213:A:ARG:HD2 | 5 | 0.17 |
| (1,1475) | 1:212:A:VAL:HG23 | 1:213:A:ARG:HD2 | 5 | 0.17 |
| (1,1458) | 1:52:A:LEU:HD21 | 1:53:A:PHE:H | 3 | 0.17 |
| (1,1458) | 1:52:A:LEU:HD22 | 1:53:A:PHE:H | 3 | 0.17 |
| (1,1458) | 1:52:A:LEU:HD23 | 1:53:A:PHE:H | 3 | 0.17 |
| (1,1436) | 1:2:A:GLN:HA | 1:86:A:ILE:HG21 | 17 | 0.17 |
| (1,1436) | 1:2:A:GLN:HA | 1:86:A:ILE:HG22 | 17 | 0.17 |
| (1,1436) | 1:2:A:GLN:HA | 1:86:A:ILE:HG23 | 17 | 0.17 |
| (1,1400) | 1:6:A:MET:HA | 1:7:A:GLU:HA | 4 | 0.17 |
| (1,1400) | 1:6:A:MET:HA | 1:7:A:GLU:HA | 16 | 0.17 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 14 | 0.17 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 14 | 0.17 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 14 | 0.17 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 2 | 0.17 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 18 | 0.17 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 6 | 0.17 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 16 | 0.17 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 2 | 0.17 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 9 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG11 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG12 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG13 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG21 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG22 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG23 | 19 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG11 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG12 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG13 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG21 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG22 | 19 | 0.17 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG23 | 19 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE1 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE2 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG21 | 1:179:A:MET:HE3 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE1 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE2 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG22 | 1:179:A:MET:HE3 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE1 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE2 | 17 | 0.17 |
| (1,1232) | 1:67:A:ILE:HG23 | 1:179:A:MET:HE3 | 17 | 0.17 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 15 | 0.17 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 14 | 0.17 |
| (1,1080) | 1:8:A:ILE:HG12 | 1:90:A:CYS:HA | 20 | 0.17 |
| (1,1040) | 1:189:A:SER:H | 1:192:A:THR:HG21 | 19 | 0.17 |
| (1,1040) | 1:189:A:SER:H | 1:192:A:THR:HG22 | 19 | 0.17 |
| (1,1040) | 1:189:A:SER:H | 1:192:A:THR:HG23 | 19 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG21 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG22 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HG23 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG21 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG22 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HG23 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG21 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG22 | 15 | 0.17 |
| (1,1030) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HG23 | 15 | 0.17 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG11 | 12 | 0.17 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG12 | 12 | 0.17 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG13 | 12 | 0.17 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG21 | 12 | 0.17 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG22 | 12 | 0.17 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG23 | 12 | 0.17 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 4 | 0.17 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 4 | 0.17 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 15 | 0.17 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 17 | 0.17 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 17 | 0.17 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 17 | 0.17 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 17 | 0.17 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 17 | 0.17 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 17 | 0.17 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG11 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG12 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG13 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG21 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG22 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HG23 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG11 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG12 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG13 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG21 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG22 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HG23 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG11 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG12 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG13 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG21 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG22 | 11 | 0.17 |
| (1,903) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HG23 | 11 | 0.17 |
| (1,902) | 1:117:A:PHE:HD1 | 1:118:A:LEU:HA | 6 | 0.17 |
| (1,902) | 1:117:A:PHE:HD2 | 1:118:A:LEU:HA | 6 | 0.17 |
| (1,859) | 1:155:A:ASP:H | 1:155:A:ASP:HB2 | 2 | 0.17 |
| (1,859) | 1:155:A:ASP:H | 1:155:A:ASP:HB2 | 10 | 0.17 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB1 | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB2 | 10 | 0.17 |
| (1,842) | 1:83:A:LYS:H | 1:130:A:ALA:HB3 | 10 | 0.17 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 3 | 0.17 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 15 | 0.17 |
| (1,761) | 1:49:A:LEU:H | 1:165:A:PHE:HD1 | 7 | 0.17 |
| (1,761) | 1:49:A:LEU:H | 1:165:A:PHE:HD2 | 7 | 0.17 |
| (1,737) | 1:164:A:LEU:H | 1:177:A:GLY:H | 10 | 0.17 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 4 | 0.17 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 19 | 0.17 |
| (1,657) | 1:42:A:VAL:H | 1:42:A:VAL:HB | 18 | 0.17 |
| (1,637) | 1:176:A:ASP:H | 1:183:A:VAL:H | 16 | 0.17 |
| (1,632) | 1:34:A:LEU:HD11 | 1:35:A:GLU:H | 9 | 0.17 |
| (1,632) | 1:34:A:LEU:HD12 | 1:35:A:GLU:H | 9 | 0.17 |
| (1,632) | 1:34:A:LEU:HD13 | 1:35:A:GLU:H | 9 | 0.17 |
| (1,632) | 1:34:A:LEU:HD21 | 1:35:A:GLU:H | 9 | 0.17 |
| (1,632) | 1:34:A:LEU:HD22 | 1:35:A:GLU:H | 9 | 0.17 |
| (1,632) | 1:34:A:LEU:HD23 | 1:35:A:GLU:H | 9 | 0.17 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 1 | 0.17 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 6 | 0.17 |
| (1,602) | 1:130:A:ALA:HB1 | 1:134:A:GLU:H | 17 | 0.17 |
| (1,602) | 1:130:A:ALA:HB2 | 1:134:A:GLU:H | 17 | 0.17 |
| (1,602) | 1:130:A:ALA:HB3 | 1:134:A:GLU:H | 17 | 0.17 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 5 | 0.17 |
| (1,500) | 1:217:A:VAL:HG11 | 1:218:A:ALA:H | 16 | 0.17 |
| (1,500) | 1:217:A:VAL:HG12 | 1:218:A:ALA:H | 16 | 0.17 |
| (1,500) | 1:217:A:VAL:HG13 | 1:218:A:ALA:H | 16 | 0.17 |
| (1,500) | 1:217:A:VAL:HG21 | 1:218:A:ALA:H | 16 | 0.17 |
| (1,500) | 1:217:A:VAL:HG22 | 1:218:A:ALA:H | 16 | 0.17 |
| (1,500) | 1:217:A:VAL:HG23 | 1:218:A:ALA:H | 16 | 0.17 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB1 | 17 | 0.17 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB2 | 17 | 0.17 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB3 | 17 | 0.17 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 20 | 0.17 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 20 | 0.17 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 20 | 0.17 |
| (1,382) | 1:120:A:GLU:H | 1:122:A:GLU:H | 4 | 0.17 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 10 | 0.17 |
| (1,361) | 1:15:A:LYS:H | 1:15:A:LYS:HE2 | 16 | 0.17 |
| (1,297) | 1:159:A:ASN:HA | 1:160:A:PHE:H | 4 | 0.17 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 5 | 0.17 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 19 | 0.17 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 7 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 7 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 7 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 12 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 12 | 0.17 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 12 | 0.17 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD11 | 12 | 0.17 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD12 | 12 | 0.17 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD13 | 12 | 0.17 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD21 | 12 | 0.17 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD22 | 12 | 0.17 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD23 | 12 | 0.17 |
| (1,23) | 1:34:A:LEU:H | 1:34:A:LEU:HG | 10 | 0.17 |
| (1,18) | 1:18:A:TYR:HD1 | 1:19:A:ARG:H | 16 | 0.17 |
| (1,18) | 1:18:A:TYR:HD2 | 1:19:A:ARG:H | 16 | 0.17 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 2 | 0.16 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 18 | 0.16 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 5 | 0.16 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 5 | 0.16 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 10 | 0.16 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 10 | 0.16 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 10 | 0.16 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 10 | 0.16 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 10 | 0.16 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 10 | 0.16 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 10 | 0.16 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 10 | 0.16 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 4 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 4 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 4 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 4 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 4 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 4 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 18 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 18 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 18 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 18 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 18 | 0.16 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 18 | 0.16 |
| (1,2031) | 1:70:A:LEU:HD11 | 1:184:A:ASN:HA | 7 | 0.16 |
| (1,2031) | 1:70:A:LEU:HD12 | 1:184:A:ASN:HA | 7 | 0.16 |
| (1,2031) | 1:70:A:LEU:HD13 | 1:184:A:ASN:HA | 7 | 0.16 |
| (1,2031) | 1:70:A:LEU:HD21 | 1:184:A:ASN:HA | 7 | 0.16 |
| (1,2031) | 1:70:A:LEU:HD22 | 1:184:A:ASN:HA | 7 | 0.16 |
| (1,2031) | 1:70:A:LEU:HD23 | 1:184:A:ASN:HA | 7 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 5 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 5 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 5 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 5 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 5 | 0.16 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 5 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG11 | 11 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG12 | 11 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG13 | 11 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG21 | 11 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG22 | 11 | 0.16 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG23 | 11 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 3 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 3 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 3 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 3 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 3 | 0.16 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 3 | 0.16 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 11 | 0.16 |
| (1,1912) | 1:28:A:PHE:HB2 | 1:219:A:LEU:H | 8 | 0.16 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 5 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD11 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD12 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD13 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD21 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD22 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD23 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD11 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD12 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD13 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD21 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD22 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD23 | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD11 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD12 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD13 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD21 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD22 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD23 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD11 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD12 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD13 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD21 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD22 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD23 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD11 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD12 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD13 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD21 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD22 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD23 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD11 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD12 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD13 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD21 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD22 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD23 | 3 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD11 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD12 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD13 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD21 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD22 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD23 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD11 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD12 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD13 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD21 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD22 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD23 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD11 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD12 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD13 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD21 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD22 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD23 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD11 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD12 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD13 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD21 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD22 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD23 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD11 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD12 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD13 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD21 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD22 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD23 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD11 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD12 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD13 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD21 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD22 | 19 | 0.16 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD23 | 19 | 0.16 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD11 | 3 | 0.16 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD12 | 3 | 0.16 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD13 | 3 | 0.16 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD21 | 3 | 0.16 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD22 | 3 | 0.16 |
| (1,1841) | 1:10:A:PRO:HB2 | 1:13:A:LEU:HD23 | 3 | 0.16 |
| (1,1808) | 1:3:A:LEU:HD11 | 1:140:A:GLN:H | 11 | 0.16 |
| (1,1808) | 1:3:A:LEU:HD12 | 1:140:A:GLN:H | 11 | 0.16 |
| (1,1808) | 1:3:A:LEU:HD13 | 1:140:A:GLN:H | 11 | 0.16 |
| (1,1808) | 1:3:A:LEU:HD21 | 1:140:A:GLN:H | 11 | 0.16 |
| (1,1808) | 1:3:A:LEU:HD22 | 1:140:A:GLN:H | 11 | 0.16 |
| (1,1808) | 1:3:A:LEU:HD23 | 1:140:A:GLN:H | 11 | 0.16 |
| (1,1793) | 1:18:A:TYR:HD1 | 1:21:A:GLY:HA2 | 17 | 0.16 |
| (1,1793) | 1:18:A:TYR:HD2 | 1:21:A:GLY:HA2 | 17 | 0.16 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 19 | 0.16 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 19 | 0.16 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 19 | 0.16 |
| (1,1761) | 1:85:A:THR:HA | 1:86:A:ILE:HB | 13 | 0.16 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 1 | 0.16 |
| (1,1738) | 1:19:A:ARG:HG2 | 1:142:A:ALA:HA | 7 | 0.16 |
| (1,1719) | 1:7:A:GLU:HA | 1:7:A:GLU:HG2 | 4 | 0.16 |
| (1,1718) | 1:210:A:GLY:H | 1:211:A:GLU:HG2 | 14 | 0.16 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 5 | 0.16 |
| (1,1673) | 1:115:A:LYS:HE2 | 1:116:A:GLN:HA | 12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 5 | 0.16 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 5 | 0.16 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD21 | 3 | 0.16 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD22 | 3 | 0.16 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD23 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB1 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB2 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB3 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB1 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB2 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB3 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB1 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB2 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB3 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB1 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB2 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB3 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB1 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB2 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB3 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB1 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB2 | 3 | 0.16 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB3 | 3 | 0.16 |
| (1,1587) | 1:121:A:THR:HG21 | 1:129:A:ARG:HD2 | 6 | 0.16 |
| (1,1587) | 1:121:A:THR:HG22 | 1:129:A:ARG:HD2 | 6 | 0.16 |
| (1,1587) | 1:121:A:THR:HG23 | 1:129:A:ARG:HD2 | 6 | 0.16 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 14 | 0.16 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 14 | 0.16 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 14 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD11 | 1:175:A:LEU:HG | 16 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD12 | 1:175:A:LEU:HG | 16 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD13 | 1:175:A:LEU:HG | 16 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD21 | 1:175:A:LEU:HG | 16 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD22 | 1:175:A:LEU:HG | 16 | 0.16 |
| (1,1577) | 1:164:A:LEU:HD23 | 1:175:A:LEU:HG | 16 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1564) | 1:74:A:GLU:HA | 1:75:A:VAL:H | 3 | 0.16 |
| (1,1564) | 1:74:A:GLU:HA | 1:75:A:VAL:H | 9 | 0.16 |
| (1,1519) | 1:16:A:VAL:HB | 1:95:A:LEU:HB2 | 14 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD11 | 1:201:A:CYS:HB2 | 6 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD12 | 1:201:A:CYS:HB2 | 6 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD13 | 1:201:A:CYS:HB2 | 6 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD21 | 1:201:A:CYS:HB2 | 6 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD22 | 1:201:A:CYS:HB2 | 6 | 0.16 |
| (1,1483) | 1:34:A:LEU:HD23 | 1:201:A:CYS:HB2 | 6 | 0.16 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 10 | 0.16 |
| (1,1433) | 1:154:A:VAL:HG11 | 1:156:A:ASP:HA | 16 | 0.16 |
| (1,1433) | 1:154:A:VAL:HG12 | 1:156:A:ASP:HA | 16 | 0.16 |
| (1,1433) | 1:154:A:VAL:HG13 | 1:156:A:ASP:HA | 16 | 0.16 |
| (1,1433) | 1:154:A:VAL:HG21 | 1:156:A:ASP:HA | 16 | 0.16 |
| (1,1433) | 1:154:A:VAL:HG22 | 1:156:A:ASP:HA | 16 | 0.16 |
| (1,1433) | 1:154:A:VAL:HG23 | 1:156:A:ASP:HA | 16 | 0.16 |
| (1,1428) | 1:23:A:ALA:HB1 | 1:107:A:GLY:HA2 | 7 | 0.16 |
| (1,1428) | 1:23:A:ALA:HB2 | 1:107:A:GLY:HA2 | 7 | 0.16 |
| (1,1428) | 1:23:A:ALA:HB3 | 1:107:A:GLY:HA2 | 7 | 0.16 |
| (1,1428) | 1:23:A:ALA:HB1 | 1:107:A:GLY:HA2 | 17 | 0.16 |
| (1,1428) | 1:23:A:ALA:HB2 | 1:107:A:GLY:HA2 | 17 | 0.16 |
| (1,1428) | 1:23:A:ALA:HB3 | 1:107:A:GLY:HA2 | 17 | 0.16 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 10 | 0.16 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 10 | 0.16 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 10 | 0.16 |
| (1,1398) | 1:81:A:PHE:H | 1:82:A:MET:HA | 3 | 0.16 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 14 | 0.16 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 6 | 0.16 |
| (1,1306) | 1:48:A:ALA:HB1 | 1:218:A:ALA:HA | 12 | 0.16 |
| (1,1306) | 1:48:A:ALA:HB2 | 1:218:A:ALA:HA | 12 | 0.16 |
| (1,1306) | 1:48:A:ALA:HB3 | 1:218:A:ALA:HA | 12 | 0.16 |
| (1,1233) | 1:154:A:VAL:HA | 1:156:A:ASP:HB2 | 11 | 0.16 |
| (1,1233) | 1:154:A:VAL:HA | 1:156:A:ASP:HB2 | 20 | 0.16 |
| (1,1189) | 1:34:A:LEU:H | 1:38:A:SER:HB2 | 13 | 0.16 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 7 | 0.16 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 15 | 0.16 |
| (1,1138) | 1:201:A:CYS:HB2 | 1:205:A:THR:HB | 8 | 0.16 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 4 | 0.16 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 11 | 0.16 |
| (1,1125) | 1:86:A:ILE:HD11 | 1:136:A:ASN:H | 11 | 0.16 |
| (1,1125) | 1:86:A:ILE:HD12 | 1:136:A:ASN:H | 11 | 0.16 |
| (1,1125) | 1:86:A:ILE:HD13 | 1:136:A:ASN:H | 11 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 3 | 0.16 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 15 | 0.16 |
| (1,1112) | 1:151:A:GLN:HA | 1:151:A:GLN:HG2 | 6 | 0.16 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD11 | 9 | 0.16 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD12 | 9 | 0.16 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD13 | 9 | 0.16 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 5 | 0.16 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 5 | 0.16 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 5 | 0.16 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 6 | 0.16 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 6 | 0.16 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 6 | 0.16 |
| (1,999) | 1:15:A:LYS:H | 1:16:A:VAL:HA | 12 | 0.16 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 3 | 0.16 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 3 | 0.16 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 3 | 0.16 |
| (1,986) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HA | 17 | 0.16 |
| (1,986) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HA | 17 | 0.16 |
| (1,986) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HA | 17 | 0.16 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG11 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG12 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG13 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG21 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG22 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE1 | 1:146:A:VAL:HG23 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG11 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG12 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG13 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG21 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG22 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE2 | 1:146:A:VAL:HG23 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG11 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG12 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG13 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG21 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG22 | 12 | 0.16 |
| (1,972) | 1:12:A:MET:HE3 | 1:146:A:VAL:HG23 | 12 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 1 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 15 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 16 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 16 | 0.16 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 16 | 0.16 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 19 | 0.16 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 6 | 0.16 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 6 | 0.16 |
| (1,911) | 1:137:A:GLU:HA | 1:140:A:GLN:H | 20 | 0.16 |
| (1,909) | 1:209:A:GLN:H | 1:209:A:GLN:HG2 | 3 | 0.16 |
| (1,909) | 1:209:A:GLN:H | 1:209:A:GLN:HG2 | 19 | 0.16 |
| (1,906) | 1:153:A:ARG:HB2 | 1:153:A:ARG:HD2 | 12 | 0.16 |
| (1,879) | 1:8:A:ILE:HG21 | 1:216:A:ALA:H | 1 | 0.16 |
| (1,879) | 1:8:A:ILE:HG22 | 1:216:A:ALA:H | 1 | 0.16 |
| (1,879) | 1:8:A:ILE:HG23 | 1:216:A:ALA:H | 1 | 0.16 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD11 | 19 | 0.16 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD12 | 19 | 0.16 |
| (1,811) | 1:93:A:ILE:HA | 1:96:A:ILE:HD13 | 19 | 0.16 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 8 | 0.16 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 16 | 0.16 |
| (1,737) | 1:164:A:LEU:H | 1:177:A:GLY:H | 17 | 0.16 |
| (1,731) | 1:194:A:LEU:H | 1:196:A:ASP:H | 11 | 0.16 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 16 | 0.16 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD1 | 1 | 0.16 |
| (1,722) | 1:86:A:ILE:H | 1:133:A:PHE:HD2 | 1 | 0.16 |
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 19 | 0.16 |
| (1,706) | 1:73:A:GLN:HA | 1:74:A:GLU:H | 17 | 0.16 |
| (1,694) | 1:206:A:GLU:HA | 1:208:A:GLU:H | 13 | 0.16 |
| (1,681) | 1:194:A:LEU:HA | 1:197:A:ALA:H | 17 | 0.16 |
| (1,662) | 1:173:A:TYR:HD1 | 1:184:A:ASN:HD22 | 7 | 0.16 |
| (1,662) | 1:173:A:TYR:HD2 | 1:184:A:ASN:HD22 | 7 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 16 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 16 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 16 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 18 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 18 | 0.16 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 18 | 0.16 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 9 | 0.16 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 8 | 0.16 |
| (1,630) | 1:112:A:SER:HA | 1:114:A:LEU:H | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,604) | 1:124:A:MET:H | 1:125:A:SER:H | 17 | 0.16 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 20 | 0.16 |
| (1,524) | 1:65:A:LYS:HA | 1:69:A:GLU:H | 18 | 0.16 |
| (1,520) | 1:17:A:LEU:H | 1:19:A:ARG:H | 17 | 0.16 |
| (1,512) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 3 | 0.16 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 7 | 0.16 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 7 | 0.16 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 7 | 0.16 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 4 | 0.16 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 4 | 0.16 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 4 | 0.16 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 15 | 0.16 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 13 | 0.16 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE1 | 3 | 0.16 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE2 | 3 | 0.16 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE3 | 3 | 0.16 |
| (1,246) | 1:164:A:LEU:HD11 | 1:175:A:LEU:H | 16 | 0.16 |
| (1,246) | 1:164:A:LEU:HD12 | 1:175:A:LEU:H | 16 | 0.16 |
| (1,246) | 1:164:A:LEU:HD13 | 1:175:A:LEU:H | 16 | 0.16 |
| (1,246) | 1:164:A:LEU:HD21 | 1:175:A:LEU:H | 16 | 0.16 |
| (1,246) | 1:164:A:LEU:HD22 | 1:175:A:LEU:H | 16 | 0.16 |
| (1,246) | 1:164:A:LEU:HD23 | 1:175:A:LEU:H | 16 | 0.16 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 3 | 0.16 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 1 | 0.16 |
| (1,190) | 1:193:A:LEU:HD11 | 1:194:A:LEU:H | 12 | 0.16 |
| (1,190) | 1:193:A:LEU:HD12 | 1:194:A:LEU:H | 12 | 0.16 |
| (1,190) | 1:193:A:LEU:HD13 | 1:194:A:LEU:H | 12 | 0.16 |
| (1,190) | 1:193:A:LEU:HD21 | 1:194:A:LEU:H | 12 | 0.16 |
| (1,190) | 1:193:A:LEU:HD22 | 1:194:A:LEU:H | 12 | 0.16 |
| (1,190) | 1:193:A:LEU:HD23 | 1:194:A:LEU:H | 12 | 0.16 |
| (1,120) | 1:80:A:TYR:HB2 | 1:101:A:ASN:H | 7 | 0.16 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 8 | 0.16 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 19 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD11 | 2 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD12 | 2 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD13 | 2 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD21 | 2 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD22 | 2 | 0.16 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD23 | 2 | 0.16 |
| (1,62) | 1:38:A:SER:HA | 1:40:A:GLY:H | 6 | 0.16 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 3 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 11 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 11 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 11 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 11 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 11 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 14 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 14 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 14 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 14 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 14 | 0.15 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 14 | 0.15 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 18 | 0.15 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 18 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 13 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 13 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 13 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 13 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 13 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 13 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 14 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 14 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 14 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 14 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 14 | 0.15 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 10 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 14 | 0.15 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 14 | 0.15 |
| (1,2241) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HB2 | 16 | 0.15 |
| (1,2241) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HB2 | 16 | 0.15 |
| (1,2241) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HB2 | 16 | 0.15 |
| (1,2241) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HB2 | 16 | 0.15 |
| (1,2241) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HB2 | 16 | 0.15 |
| (1,2241) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HB2 | 16 | 0.15 |
| (1,2202) | 1:136:A:ASN:H | 1:140:A:GLN:HE21 | 5 | 0.15 |
| (1,2202) | 1:136:A:ASN:H | 1:140:A:GLN:HE22 | 5 | 0.15 |
| (1,2193) | 1:131:A:LYS:H | 1:132:A:CYS:HB2 | 2 | 0.15 |
| (1,2098) | 1:99:A:VAL:HA | 1:102:A:ASN:HD21 | 12 | 0.15 |
| (1,2098) | 1:99:A:VAL:HA | 1:102:A:ASN:HD22 | 12 | 0.15 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 7 | 0.15 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 7 | 0.15 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 7 | 0.15 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 7 | 0.15 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 7 | 0.15 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 7 | 0.15 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 19 | 0.15 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 19 | 0.15 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 19 | 0.15 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 19 | 0.15 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 19 | 0.15 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 19 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 7 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 7 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 7 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 7 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 7 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 7 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 9 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 9 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 9 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 9 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 9 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 12 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 12 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 12 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 12 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 12 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 12 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 14 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 14 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 14 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 14 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 14 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 14 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 17 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 17 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 17 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 17 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 17 | 0.15 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 17 | 0.15 |
| (1,1963) | 1:49:A:LEU:HD11 | 1:201:A:CYS:HB2 | 17 | 0.15 |
| (1,1963) | 1:49:A:LEU:HD12 | 1:201:A:CYS:HB2 | 17 | 0.15 |
| (1,1963) | 1:49:A:LEU:HD13 | 1:201:A:CYS:HB2 | 17 | 0.15 |
| (1,1963) | 1:49:A:LEU:HD21 | 1:201:A:CYS:HB2 | 17 | 0.15 |
| (1,1963) | 1:49:A:LEU:HD22 | 1:201:A:CYS:HB2 | 17 | 0.15 |
| (1,1963) | 1:49:A:LEU:HD23 | 1:201:A:CYS:HB2 | 17 | 0.15 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 5 | 0.15 |
| (1,1932) | 1:36:A:GLU:HG2 | 1:37:A:GLU:H | 7 | 0.15 |
| (1,1920) | 1:33:A:GLY:H | 1:194:A:LEU:HD11 | 7 | 0.15 |
| (1,1920) | 1:33:A:GLY:H | 1:194:A:LEU:HD12 | 7 | 0.15 |
| (1,1920) | 1:33:A:GLY:H | 1:194:A:LEU:HD13 | 7 | 0.15 |
| (1,1920) | 1:33:A:GLY:H | 1:194:A:LEU:HD21 | 7 | 0.15 |
| (1,1920) | 1:33:A:GLY:H | 1:194:A:LEU:HD22 | 7 | 0.15 |
| (1,1920) | 1:33:A:GLY:H | 1:194:A:LEU:HD23 | 7 | 0.15 |
| (1,1919) | 1:33:A:GLY:H | 1:194:A:LEU:HB2 | 18 | 0.15 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 2 | 0.15 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD11 | 3 | 0.15 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD12 | 3 | 0.15 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD13 | 3 | 0.15 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD21 | 3 | 0.15 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD22 | 3 | 0.15 |
| (1,1887) | 1:26:A:TRP:H | 1:106:A:LEU:HD23 | 3 | 0.15 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE1 | 6 | 0.15 |
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE2 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1820) | 1:6:A:MET:HB2 | 1:12:A:MET:HE3 | 6 | 0.15 |
| (1,1805) | 1:3:A:LEU:HD11 | 1:86:A:ILE:HB | 19 | 0.15 |
| (1,1805) | 1:3:A:LEU:HD12 | 1:86:A:ILE:HB | 19 | 0.15 |
| (1,1805) | 1:3:A:LEU:HD13 | 1:86:A:ILE:HB | 19 | 0.15 |
| (1,1805) | 1:3:A:LEU:HD21 | 1:86:A:ILE:HB | 19 | 0.15 |
| (1,1805) | 1:3:A:LEU:HD22 | 1:86:A:ILE:HB | 19 | 0.15 |
| (1,1805) | 1:3:A:LEU:HD23 | 1:86:A:ILE:HB | 19 | 0.15 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 11 | 0.15 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 11 | 0.15 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 18 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE1 | 1 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE2 | 1 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE3 | 1 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE1 | 8 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE2 | 8 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE3 | 8 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE1 | 17 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE2 | 17 | 0.15 |
| (1,1750) | 1:121:A:THR:HB | 1:124:A:MET:HE3 | 17 | 0.15 |
| (1,1688) | 1:7:A:GLU:HA | 1:9:A:ASN:HB2 | 1 | 0.15 |
| (1,1651) | 1:31:A:VAL:HG11 | 1:49:A:LEU:HG | 9 | 0.15 |
| (1,1651) | 1:31:A:VAL:HG12 | 1:49:A:LEU:HG | 9 | 0.15 |
| (1,1651) | 1:31:A:VAL:HG13 | 1:49:A:LEU:HG | 9 | 0.15 |
| (1,1651) | 1:31:A:VAL:HG21 | 1:49:A:LEU:HG | 9 | 0.15 |
| (1,1651) | 1:31:A:VAL:HG22 | 1:49:A:LEU:HG | 9 | 0.15 |
| (1,1651) | 1:31:A:VAL:HG23 | 1:49:A:LEU:HG | 9 | 0.15 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD21 | 20 | 0.15 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD22 | 20 | 0.15 |
| (1,1616) | 1:32:A:LEU:H | 1:32:A:LEU:HD23 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB1 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB2 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB3 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB1 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB2 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB3 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB1 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB2 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB3 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB1 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB2 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB3 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB1 | 20 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB2 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB3 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB1 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB2 | 20 | 0.15 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB3 | 20 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 1 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 1 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 1 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 3 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 3 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 3 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 7 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 7 | 0.15 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 7 | 0.15 |
| (1,1564) | 1:74:A:GLU:HA | 1:75:A:VAL:H | 14 | 0.15 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 10 | 0.15 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 17 | 0.15 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 3 | 0.15 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 6 | 0.15 |
| (1,1543) | 1:144:A:ASP:HA | 1:146:A:VAL:H | 16 | 0.15 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 18 | 0.15 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 18 | 0.15 |
| (1,1535) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 18 | 0.15 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 4 | 0.15 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 4 | 0.15 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 4 | 0.15 |
| (1,1493) | 1:207:A:ARG:HA | 1:207:A:ARG:HD2 | 11 | 0.15 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 13 | 0.15 |
| (1,1481) | 1:121:A:THR:HG21 | 1:124:A:MET:HG2 | 6 | 0.15 |
| (1,1481) | 1:121:A:THR:HG22 | 1:124:A:MET:HG2 | 6 | 0.15 |
| (1,1481) | 1:121:A:THR:HG23 | 1:124:A:MET:HG2 | 6 | 0.15 |
| (1,1443) | 1:212:A:VAL:HA | 1:213:A:ARG:HB2 | 9 | 0.15 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 13 | 0.15 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 13 | 0.15 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 13 | 0.15 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 4 | 0.15 |
| (1,1412) | 1:77:A:PRO:HG2 | 1:78:A:LYS:HD2 | 15 | 0.15 |
| (1,1398) | 1:81:A:PHE:H | 1:82:A:MET:HA | 13 | 0.15 |
| (1,1362) | 1:32:A:LEU:HB2 | 1:38:A:SER:HA | 16 | 0.15 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 9 | 0.15 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 15 | 0.15 |
| (1,1352) | 1:133:A:PHE:HA | 1:135:A:LYS:H | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 14 | 0.15 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 10 | 0.15 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 10 | 0.15 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 10 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD11 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD12 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD13 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD21 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD22 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD11 | 1:164:A:LEU:HD23 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD11 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD12 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD13 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD21 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD22 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD12 | 1:164:A:LEU:HD23 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD11 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD12 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD13 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD21 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD22 | 2 | 0.15 |
| (1,1281) | 1:163:A:ILE:HD13 | 1:164:A:LEU:HD23 | 2 | 0.15 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 10 | 0.15 |
| (1,1258) | 1:56:A:THR:HB | 1:58:A:GLN:HA | 11 | 0.15 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD11 | 9 | 0.15 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD12 | 9 | 0.15 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD13 | 9 | 0.15 |
| (1,1211) | 1:52:A:LEU:HA | 1:215:A:SER:HB2 | 7 | 0.15 |
| (1,1210) | 1:215:A:SER:HB2 | 1:216:A:ALA:H | 15 | 0.15 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG21 | 8 | 0.15 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG22 | 8 | 0.15 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG23 | 8 | 0.15 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD1 | 12 | 0.15 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD2 | 12 | 0.15 |
| (1,1204) | 1:75:A:VAL:HG11 | 1:76:A:SER:HA | 6 | 0.15 |
| (1,1204) | 1:75:A:VAL:HG12 | 1:76:A:SER:HA | 6 | 0.15 |
| (1,1204) | 1:75:A:VAL:HG13 | 1:76:A:SER:HA | 6 | 0.15 |
| (1,1204) | 1:75:A:VAL:HG21 | 1:76:A:SER:HA | 6 | 0.15 |
| (1,1204) | 1:75:A:VAL:HG22 | 1:76:A:SER:HA | 6 | 0.15 |
| (1,1204) | 1:75:A:VAL:HG23 | 1:76:A:SER:HA | 6 | 0.15 |
| (1,1200) | 1:5:A:PRO:HA | 1:88:A:ASN:HB2 | 20 | 0.15 |
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1172) | 1:146:A:VAL:HA | 1:149:A:GLU:HB2 | 12 | 0.15 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 6 | 0.15 |
| (1,1157) | 1:28:A:PHE:HA | 1:217:A:VAL:HA | 13 | 0.15 |
| (1,1112) | 1:151:A:GLN:HA | 1:151:A:GLN:HG2 | 8 | 0.15 |
| (1,1112) | 1:151:A:GLN:HA | 1:151:A:GLN:HG2 | 19 | 0.15 |
| (1,1093) | 1:197:A:ALA:HB1 | 1:201:A:CYS:HB2 | 9 | 0.15 |
| (1,1093) | 1:197:A:ALA:HB2 | 1:201:A:CYS:HB2 | 9 | 0.15 |
| (1,1093) | 1:197:A:ALA:HB3 | 1:201:A:CYS:HB2 | 9 | 0.15 |
| (1,1067) | 1:117:A:PHE:HD1 | 1:139:A:ILE:HG12 | 14 | 0.15 |
| (1,1067) | 1:117:A:PHE:HD2 | 1:139:A:ILE:HG12 | 14 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG11 | 1:138:A:ALA:HB1 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG11 | 1:138:A:ALA:HB2 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG11 | 1:138:A:ALA:HB3 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG12 | 1:138:A:ALA:HB1 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG12 | 1:138:A:ALA:HB2 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG12 | 1:138:A:ALA:HB3 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG13 | 1:138:A:ALA:HB1 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG13 | 1:138:A:ALA:HB2 | 9 | 0.15 |
| (1,1044) | 1:113:A:VAL:HG13 | 1:138:A:ALA:HB3 | 9 | 0.15 |
| (1,1019) | 1:117:A:PHE:HB2 | 1:118:A:LEU:HA | 18 | 0.15 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE1 | 15 | 0.15 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE2 | 15 | 0.15 |
| (1,969) | 1:7:A:GLU:H | 1:12:A:MET:HE3 | 15 | 0.15 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 18 | 0.15 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 18 | 0.15 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 11 | 0.15 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 18 | 0.15 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 18 | 0.15 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG11 | 17 | 0.15 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG12 | 17 | 0.15 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG13 | 17 | 0.15 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG21 | 17 | 0.15 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG22 | 17 | 0.15 |
| (1,925) | 1:17:A:LEU:HA | 1:22:A:VAL:HG23 | 17 | 0.15 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD11 | 10 | 0.15 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD12 | 10 | 0.15 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD13 | 10 | 0.15 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD21 | 10 | 0.15 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD22 | 10 | 0.15 |
| (1,918) | 1:167:A:ASN:H | 1:193:A:LEU:HD23 | 10 | 0.15 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 13 | 0.15 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 13 | 0.15 |
| (1,896) | 1:26:A:TRP:HH2 | 1:221:A:LYS:HA | 13 | 0.15 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD1 | 5 | 0.15 |
| (1,892) | 1:96:A:ILE:HG21 | 1:117:A:PHE:HD2 | 5 | 0.15 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD1 | 5 | 0.15 |
| (1,892) | 1:96:A:ILE:HG22 | 1:117:A:PHE:HD2 | 5 | 0.15 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD1 | 5 | 0.15 |
| (1,892) | 1:96:A:ILE:HG23 | 1:117:A:PHE:HD2 | 5 | 0.15 |
| (1,815) | 1:93:A:ILE:HG21 | 1:164:A:LEU:HA | 13 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,815) | 1:93:A:ILE:HG22 | 1:164:A:LEU:HA | 13 | 0.15 |
| (1,815) | 1:93:A:ILE:HG23 | 1:164:A:LEU:HA | 13 | 0.15 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 18 | 0.15 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 12 | 0.15 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 20 | 0.15 |
| (1,738) | 1:177:A:GLY:H | 1:179:A:MET:HE1 | 7 | 0.15 |
| (1,738) | 1:177:A:GLY:H | 1:179:A:MET:HE2 | 7 | 0.15 |
| (1,738) | 1:177:A:GLY:H | 1:179:A:MET:HE3 | 7 | 0.15 |
| (1,737) | 1:164:A:LEU:H | 1:177:A:GLY:H | 18 | 0.15 |
| (1,730) | 1:26:A:TRP:HE1 | 1:107:A:GLY:H | 12 | 0.15 |
| (1,727) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE22 | 4 | 0.15 |
| (1,727) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE22 | 4 | 0.15 |
| (1,727) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE22 | 4 | 0.15 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 17 | 0.15 |
| (1,668) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 17 | 0.15 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 6 | 0.15 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 6 | 0.15 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 6 | 0.15 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 10 | 0.15 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 10 | 0.15 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 10 | 0.15 |
| (1,657) | 1:42:A:VAL:H | 1:42:A:VAL:HB | 5 | 0.15 |
| (1,630) | 1:112:A:SER:HA | 1:114:A:LEU:H | 10 | 0.15 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG11 | 11 | 0.15 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG12 | 11 | 0.15 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG13 | 11 | 0.15 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG21 | 11 | 0.15 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG22 | 11 | 0.15 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG23 | 11 | 0.15 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 12 | 0.15 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 8 | 0.15 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 18 | 0.15 |
| (1,597) | 1:96:A:ILE:H | 1:99:A:VAL:H | 17 | 0.15 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 16 | 0.15 |
| (1,558) | 1:172:A:LEU:H | 1:187:A:ALA:HA | 9 | 0.15 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 10 | 0.15 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 10 | 0.15 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 10 | 0.15 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 10 | 0.15 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 10 | 0.15 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 10 | 0.15 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 8 | 0.15 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 9 | 0.15 |
| (1,512) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 18 | 0.15 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 16 | 0.15 |
| (1,465) | 1:168:A:VAL:H | 1:173:A:TYR:HE1 | 13 | 0.15 |
| (1,465) | 1:168:A:VAL:H | 1:173:A:TYR:HE2 | 13 | 0.15 |
| (1,416) | 1:193:A:LEU:HD11 | 1:197:A:ALA:H | 14 | 0.15 |
| (1,416) | 1:193:A:LEU:HD12 | 1:197:A:ALA:H | 14 | 0.15 |
| (1,416) | 1:193:A:LEU:HD13 | 1:197:A:ALA:H | 14 | 0.15 |
| (1,416) | 1:193:A:LEU:HD21 | 1:197:A:ALA:H | 14 | 0.15 |
| (1,416) | 1:193:A:LEU:HD22 | 1:197:A:ALA:H | 14 | 0.15 |
| (1,416) | 1:193:A:LEU:HD23 | 1:197:A:ALA:H | 14 | 0.15 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 19 | 0.15 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 19 | 0.15 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 19 | 0.15 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 8 | 0.15 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 8 | 0.15 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 8 | 0.15 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 9 | 0.15 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 9 | 0.15 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 9 | 0.15 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 9 | 0.15 |
| (1,382) | 1:120:A:GLU:H | 1:122:A:GLU:H | 15 | 0.15 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 8 | 0.15 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 11 | 0.15 |
| (1,292) | 1:86:A:ILE:HD11 | 1:140:A:GLN:HE21 | 19 | 0.15 |
| (1,292) | 1:86:A:ILE:HD12 | 1:140:A:GLN:HE21 | 19 | 0.15 |
| (1,292) | 1:86:A:ILE:HD13 | 1:140:A:GLN:HE21 | 19 | 0.15 |
| (1,273) | 1:123:A:LYS:HG2 | 1:124:A:MET:H | 17 | 0.15 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 2 | 0.15 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 9 | 0.15 |
| (1,188) | 1:191:A:ASP:HB2 | 1:193:A:LEU:H | 17 | 0.15 |
| (1,175) | 1:166:A:ASN:H | 1:175:A:LEU:H | 19 | 0.15 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 12 | 0.15 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 13 | 0.15 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 10 | 0.15 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 10 | 0.15 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 10 | 0.15 |
| (1,130) | 1:110:A:ASP:H | 1:110:A:ASP:HB2 | 12 | 0.15 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 11 | 0.15 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 12 | 0.15 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 9 | 0.15 |
| (1,52) | 1:32:A:LEU:H | 1:32:A:LEU:HG | 17 | 0.15 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 7 | 0.15 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 7 | 0.15 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 7 | 0.15 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 7 | 0.15 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 7 | 0.15 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 7 | 0.15 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 5 | 0.14 |
| (1,2327) | 1:189:A:SER:HB2 | 1:190:A:GLU:HG2 | 12 | 0.14 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 5 | 0.14 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 5 | 0.14 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 5 | 0.14 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 8 | 0.14 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 8 | 0.14 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 8 | 0.14 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD11 | 12 | 0.14 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD12 | 12 | 0.14 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD13 | 12 | 0.14 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD21 | 12 | 0.14 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD22 | 12 | 0.14 |
| (1,2255) | 1:165:A:PHE:HB2 | 1:172:A:LEU:HD23 | 12 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 5 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 20 | 0.14 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 20 | 0.14 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 13 | 0.14 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 13 | 0.14 |
| (1,2232) | 1:151:A:GLN:HB2 | 1:151:A:GLN:HE21 | 9 | 0.14 |
| (1,2232) | 1:151:A:GLN:HB2 | 1:151:A:GLN:HE22 | 9 | 0.14 |
| (1,2189) | 1:124:A:MET:HE1 | 1:132:A:CYS:HB2 | 4 | 0.14 |
| (1,2189) | 1:124:A:MET:HE2 | 1:132:A:CYS:HB2 | 4 | 0.14 |
| (1,2189) | 1:124:A:MET:HE3 | 1:132:A:CYS:HB2 | 4 | 0.14 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 14 | 0.14 |
| (1,2079) | 1:82:A:MET:HE1 | 1:93:A:ILE:HG12 | 19 | 0.14 |
| (1,2079) | 1:82:A:MET:HE2 | 1:93:A:ILE:HG12 | 19 | 0.14 |
| (1,2079) | 1:82:A:MET:HE3 | 1:93:A:ILE:HG12 | 19 | 0.14 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 16 | 0.14 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 16 | 0.14 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 16 | 0.14 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 16 | 0.14 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 16 | 0.14 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 16 | 0.14 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 4 | 0.14 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 4 | 0.14 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 4 | 0.14 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 4 | 0.14 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 4 | 0.14 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 4 | 0.14 |
| (1,2009) | 1:58:A:GLN:HB2 | 1:61:A:ASN:HD21 | 8 | 0.14 |
| (1,2009) | 1:58:A:GLN:HB2 | 1:61:A:ASN:HD22 | 8 | 0.14 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE21 | 9 | 0.14 |
| (1,1999) | 1:56:A:THR:HB | 1:58:A:GLN:HE22 | 9 | 0.14 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 13 | 0.14 |
| (1,1927) | 1:36:A:GLU:H | 1:36:A:GLU:HG2 | 8 | 0.14 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 4 | 0.14 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 4 | 0.14 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 4 | 0.14 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 4 | 0.14 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 4 | 0.14 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 4 | 0.14 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD11 | 7 | 0.14 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD12 | 7 | 0.14 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD13 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD21 | 7 | 0.14 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD22 | 7 | 0.14 |
| (1,1870) | 1:17:A:LEU:HA | 1:95:A:LEU:HD23 | 7 | 0.14 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB1 | 17 | 0.14 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB2 | 17 | 0.14 |
| (1,1822) | 1:6:A:MET:HB2 | 1:147:A:ALA:HB3 | 17 | 0.14 |
| (1,1814) | 1:3:A:LEU:HD11 | 1:143:A:HIS:H | 5 | 0.14 |
| (1,1814) | 1:3:A:LEU:HD12 | 1:143:A:HIS:H | 5 | 0.14 |
| (1,1814) | 1:3:A:LEU:HD13 | 1:143:A:HIS:H | 5 | 0.14 |
| (1,1814) | 1:3:A:LEU:HD21 | 1:143:A:HIS:H | 5 | 0.14 |
| (1,1814) | 1:3:A:LEU:HD22 | 1:143:A:HIS:H | 5 | 0.14 |
| (1,1814) | 1:3:A:LEU:HD23 | 1:143:A:HIS:H | 5 | 0.14 |
| (1,1794) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HB | 15 | 0.14 |
| (1,1794) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HB | 15 | 0.14 |
| (1,1788) | 1:14:A:ASN:HB2 | 1:18:A:TYR:HE1 | 9 | 0.14 |
| (1,1788) | 1:14:A:ASN:HB2 | 1:18:A:TYR:HE2 | 9 | 0.14 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE1 | 2 | 0.14 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE2 | 2 | 0.14 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 4 | 0.14 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 4 | 0.14 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 4 | 0.14 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 12 | 0.14 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 12 | 0.14 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 12 | 0.14 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 4 | 0.14 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 8 | 0.14 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 8 | 0.14 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 8 | 0.14 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 15 | 0.14 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 15 | 0.14 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 15 | 0.14 |
| (1,1662) | 1:21:A:GLY:HA2 | 1:108:A:PHE:HB2 | 5 | 0.14 |
| (1,1629) | 1:131:A:LYS:HA | 1:135:A:LYS:HG2 | 7 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG11 | 1:81:A:PHE:HE1 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG11 | 1:81:A:PHE:HE2 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG12 | 1:81:A:PHE:HE1 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG12 | 1:81:A:PHE:HE2 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG13 | 1:81:A:PHE:HE1 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG13 | 1:81:A:PHE:HE2 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG21 | 1:81:A:PHE:HE1 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG21 | 1:81:A:PHE:HE2 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG22 | 1:81:A:PHE:HE1 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1594) | 1:75:A:VAL:HG22 | 1:81:A:PHE:HE2 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG23 | 1:81:A:PHE:HE1 | 10 | 0.14 |
| (1,1594) | 1:75:A:VAL:HG23 | 1:81:A:PHE:HE2 | 10 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 6 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 6 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 6 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 8 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 8 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 8 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 11 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 11 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 11 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 19 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 19 | 0.14 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 19 | 0.14 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 1 | 0.14 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 1 | 0.14 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 1 | 0.14 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE1 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE2 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG21 | 1:124:A:MET:HE3 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE1 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE2 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG22 | 1:124:A:MET:HE3 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE1 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE2 | 2 | 0.14 |
| (1,1497) | 1:121:A:THR:HG23 | 1:124:A:MET:HE3 | 2 | 0.14 |
| (1,1465) | 1:212:A:VAL:HB | 1:213:A:ARG:HD2 | 1 | 0.14 |
| (1,1434) | 1:156:A:ASP:HA | 1:157:A:LYS:HA | 5 | 0.14 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 20 | 0.14 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 20 | 0.14 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 20 | 0.14 |
| (1,1366) | 1:117:A:PHE:H | 1:118:A:LEU:HA | 19 | 0.14 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 8 | 0.14 |
| (1,1338) | 1:80:A:TYR:HE1 | 1:122:A:GLU:HA | 19 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG11 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG12 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG13 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG21 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG22 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG23 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG11 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG12 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG13 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG21 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG22 | 8 | 0.14 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG23 | 8 | 0.14 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG21 | 1 | 0.14 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG22 | 1 | 0.14 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG23 | 1 | 0.14 |
| (1,1175) | 1:77:A:PRO:HA | 1:78:A:LYS:HD2 | 20 | 0.14 |
| (1,1163) | 1:92:A:THR:HB | 1:93:A:ILE:HA | 2 | 0.14 |
| (1,1163) | 1:92:A:THR:HB | 1:93:A:ILE:HA | 10 | 0.14 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 17 | 0.14 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD11 | 7 | 0.14 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD12 | 7 | 0.14 |
| (1,1106) | 1:133:A:PHE:HA | 1:139:A:ILE:HD13 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB1 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB2 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD11 | 1:130:A:ALA:HB3 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB1 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB2 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD12 | 1:130:A:ALA:HB3 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB1 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB2 | 7 | 0.14 |
| (1,1100) | 1:86:A:ILE:HD13 | 1:130:A:ALA:HB3 | 7 | 0.14 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 7 | 0.14 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 7 | 0.14 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 7 | 0.14 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 1 | 0.14 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 6 | 0.14 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 7 | 0.14 |
| (1,1056) | 1:52:A:LEU:HB2 | 1:214:A:PHE:HD1 | 5 | 0.14 |
| (1,1056) | 1:52:A:LEU:HB2 | 1:214:A:PHE:HD2 | 5 | 0.14 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 11 | 0.14 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 16 | 0.14 |
| (1,962) | 1:124:A:MET:HE1 | 1:129:A:ARG:H | 9 | 0.14 |
| (1,962) | 1:124:A:MET:HE2 | 1:129:A:ARG:H | 9 | 0.14 |
| (1,962) | 1:124:A:MET:HE3 | 1:129:A:ARG:H | 9 | 0.14 |
| (1,958) | 1:79:A:VAL:H | 1:168:A:VAL:HG11 | 7 | 0.14 |
| (1,958) | 1:79:A:VAL:H | 1:168:A:VAL:HG12 | 7 | 0.14 |
| (1,958) | 1:79:A:VAL:H | 1:168:A:VAL:HG13 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 7 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 13 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 20 | 0.14 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 20 | 0.14 |
| (1,946) | 1:31:A:VAL:HG11 | 1:218:A:ALA:H | 13 | 0.14 |
| (1,946) | 1:31:A:VAL:HG12 | 1:218:A:ALA:H | 13 | 0.14 |
| (1,946) | 1:31:A:VAL:HG13 | 1:218:A:ALA:H | 13 | 0.14 |
| (1,946) | 1:31:A:VAL:HG21 | 1:218:A:ALA:H | 13 | 0.14 |
| (1,946) | 1:31:A:VAL:HG22 | 1:218:A:ALA:H | 13 | 0.14 |
| (1,946) | 1:31:A:VAL:HG23 | 1:218:A:ALA:H | 13 | 0.14 |
| (1,939) | 1:98:A:ALA:HA | 1:101:A:ASN:H | 12 | 0.14 |
| (1,930) | 1:92:A:THR:HG21 | 1:96:A:ILE:H | 3 | 0.14 |
| (1,930) | 1:92:A:THR:HG22 | 1:96:A:ILE:H | 3 | 0.14 |
| (1,930) | 1:92:A:THR:HG23 | 1:96:A:ILE:H | 3 | 0.14 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 2 | 0.14 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 2 | 0.14 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 2 | 0.14 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 2 | 0.14 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 2 | 0.14 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 2 | 0.14 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 1 | 0.14 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 1 | 0.14 |
| (1,915) | 1:80:A:TYR:HD1 | 1:122:A:GLU:HA | 2 | 0.14 |
| (1,915) | 1:80:A:TYR:HD2 | 1:122:A:GLU:HA | 2 | 0.14 |
| (1,871) | 1:221:A:LYS:HA | 1:221:A:LYS:HE2 | 13 | 0.14 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 2 | 0.14 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 2 | 0.14 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 2 | 0.14 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 2 | 0.14 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 2 | 0.14 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 10 | 0.14 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 17 | 0.14 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 10 | 0.14 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 10 | 0.14 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 10 | 0.14 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 4 | 0.14 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 4 | 0.14 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 4 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG11 | 19 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG12 | 19 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG13 | 19 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG21 | 19 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG22 | 19 | 0.14 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG23 | 19 | 0.14 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 1 | 0.14 |
| (1,603) | 1:14:A:ASN:H | 1:28:A:PHE:H | 8 | 0.14 |
| (1,590) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 2 | 0.14 |
| (1,590) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 13 | 0.14 |
| (1,541) | 1:3:A:LEU:HD21 | 1:143:A:HIS:H | 2 | 0.14 |
| (1,541) | 1:3:A:LEU:HD22 | 1:143:A:HIS:H | 2 | 0.14 |
| (1,541) | 1:3:A:LEU:HD23 | 1:143:A:HIS:H | 2 | 0.14 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 8 | 0.14 |
| (1,512) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 10 | 0.14 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD11 | 16 | 0.14 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD12 | 16 | 0.14 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD13 | 16 | 0.14 |
| (1,447) | 1:136:A:ASN:H | 1:140:A:GLN:HB2 | 10 | 0.14 |
| (1,429) | 1:122:A:GLU:H | 1:124:A:MET:H | 9 | 0.14 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 7 | 0.14 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 7 | 0.14 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 7 | 0.14 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 7 | 0.14 |
| (1,317) | 1:206:A:GLU:H | 1:208:A:GLU:H | 2 | 0.14 |
| (1,305) | 1:31:A:VAL:H | 1:217:A:VAL:H | 15 | 0.14 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE1 | 8 | 0.14 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE2 | 8 | 0.14 |
| (1,264) | 1:64:A:LYS:H | 1:179:A:MET:HE3 | 8 | 0.14 |
| (1,254) | 1:209:A:GLN:HG2 | 1:210:A:GLY:H | 20 | 0.14 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 6 | 0.14 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 6 | 0.14 |
| (1,122) | 1:99:A:VAL:HG11 | 1:102:A:ASN:H | 5 | 0.14 |
| (1,122) | 1:99:A:VAL:HG12 | 1:102:A:ASN:H | 5 | 0.14 |
| (1,122) | 1:99:A:VAL:HG13 | 1:102:A:ASN:H | 5 | 0.14 |
| (1,122) | 1:99:A:VAL:HG21 | 1:102:A:ASN:H | 5 | 0.14 |
| (1,122) | 1:99:A:VAL:HG22 | 1:102:A:ASN:H | 5 | 0.14 |
| (1,122) | 1:99:A:VAL:HG23 | 1:102:A:ASN:H | 5 | 0.14 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 6 | 0.14 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 8 | 0.14 |
| (1,43) | 1:28:A:PHE:H | 1:29:A:VAL:HG11 | 16 | 0.14 |
| (1,43) | 1:28:A:PHE:H | 1:29:A:VAL:HG12 | 16 | 0.14 |
| (1,43) | 1:28:A:PHE:H | 1:29:A:VAL:HG13 | 16 | 0.14 |
| (1,43) | 1:28:A:PHE:H | 1:29:A:VAL:HG21 | 16 | 0.14 |
| (1,43) | 1:28:A:PHE:H | 1:29:A:VAL:HG22 | 16 | 0.14 |
| (1,43) | 1:28:A:PHE:H | 1:29:A:VAL:HG23 | 16 | 0.14 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 10 | 0.14 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 10 | 0.14 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 10 | 0.14 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 10 | 0.14 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 10 | 0.14 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 10 | 0.14 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 18 | 0.14 |
| (1,18) | 1:18:A:TYR:HD1 | 1:19:A:ARG:H | 9 | 0.14 |
| (1,18) | 1:18:A:TYR:HD2 | 1:19:A:ARG:H | 9 | 0.14 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 13 | 0.13 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 16 | 0.13 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG11 | 7 | 0.13 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG12 | 7 | 0.13 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG13 | 7 | 0.13 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG21 | 7 | 0.13 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG22 | 7 | 0.13 |
| (1,2338) | 1:197:A:ALA:HA | 1:200:A:VAL:HG23 | 7 | 0.13 |
| (1,2317) | 1:179:A:MET:HE1 | 1:181:A:PHE:HB2 | 3 | 0.13 |
| (1,2317) | 1:179:A:MET:HE2 | 1:181:A:PHE:HB2 | 3 | 0.13 |
| (1,2317) | 1:179:A:MET:HE3 | 1:181:A:PHE:HB2 | 3 | 0.13 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 19 | 0.13 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 19 | 0.13 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 19 | 0.13 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 19 | 0.13 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 19 | 0.13 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 19 | 0.13 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 12 | 0.13 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 12 | 0.13 |
| (1,2271) | 1:167:A:ASN:HB2 | 1:170:A:GLY:H | 19 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HB2 | 9 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HB2 | 9 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HB2 | 9 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HB2 | 9 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HB2 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2241) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HB2 | 9 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HB2 | 19 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HB2 | 19 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HB2 | 19 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HB2 | 19 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HB2 | 19 | 0.13 |
| (1,2241) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HB2 | 19 | 0.13 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD21 | 7 | 0.13 |
| (1,2239) | 1:158:A:VAL:HA | 1:159:A:ASN:HD22 | 7 | 0.13 |
| (1,2195) | 1:132:A:CYS:HB2 | 1:135:A:LYS:HD2 | 16 | 0.13 |
| (1,2147) | 1:113:A:VAL:HG11 | 1:114:A:LEU:H | 16 | 0.13 |
| (1,2147) | 1:113:A:VAL:HG12 | 1:114:A:LEU:H | 16 | 0.13 |
| (1,2147) | 1:113:A:VAL:HG13 | 1:114:A:LEU:H | 16 | 0.13 |
| (1,2147) | 1:113:A:VAL:HG21 | 1:114:A:LEU:H | 16 | 0.13 |
| (1,2147) | 1:113:A:VAL:HG22 | 1:114:A:LEU:H | 16 | 0.13 |
| (1,2147) | 1:113:A:VAL:HG23 | 1:114:A:LEU:H | 16 | 0.13 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 6 | 0.13 |
| (1,2058) | 1:79:A:VAL:HG11 | 1:81:A:PHE:H | 6 | 0.13 |
| (1,2058) | 1:79:A:VAL:HG12 | 1:81:A:PHE:H | 6 | 0.13 |
| (1,2058) | 1:79:A:VAL:HG13 | 1:81:A:PHE:H | 6 | 0.13 |
| (1,2058) | 1:79:A:VAL:HG21 | 1:81:A:PHE:H | 6 | 0.13 |
| (1,2058) | 1:79:A:VAL:HG22 | 1:81:A:PHE:H | 6 | 0.13 |
| (1,2058) | 1:79:A:VAL:HG23 | 1:81:A:PHE:H | 6 | 0.13 |
| (1,2049) | 1:76:A:SER:HB2 | 1:79:A:VAL:HG11 | 17 | 0.13 |
| (1,2049) | 1:76:A:SER:HB2 | 1:79:A:VAL:HG12 | 17 | 0.13 |
| (1,2049) | 1:76:A:SER:HB2 | 1:79:A:VAL:HG13 | 17 | 0.13 |
| (1,2049) | 1:76:A:SER:HB2 | 1:79:A:VAL:HG21 | 17 | 0.13 |
| (1,2049) | 1:76:A:SER:HB2 | 1:79:A:VAL:HG22 | 17 | 0.13 |
| (1,2049) | 1:76:A:SER:HB2 | 1:79:A:VAL:HG23 | 17 | 0.13 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 8 | 0.13 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 8 | 0.13 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 8 | 0.13 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 8 | 0.13 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 8 | 0.13 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 8 | 0.13 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG11 | 18 | 0.13 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG12 | 18 | 0.13 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG13 | 18 | 0.13 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG21 | 18 | 0.13 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG22 | 18 | 0.13 |
| (1,2021) | 1:67:A:ILE:HA | 1:183:A:VAL:HG23 | 18 | 0.13 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 16 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 16 | 0.13 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 16 | 0.13 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 16 | 0.13 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 16 | 0.13 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 16 | 0.13 |
| (1,2018) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HD2 | 1 | 0.13 |
| (1,1993) | 1:55:A:LEU:HG | 1:161:A:HIS:HB2 | 15 | 0.13 |
| (1,1990) | 1:55:A:LEU:H | 1:161:A:HIS:HB2 | 7 | 0.13 |
| (1,1965) | 1:49:A:LEU:HD11 | 1:219:A:LEU:H | 7 | 0.13 |
| (1,1965) | 1:49:A:LEU:HD12 | 1:219:A:LEU:H | 7 | 0.13 |
| (1,1965) | 1:49:A:LEU:HD13 | 1:219:A:LEU:H | 7 | 0.13 |
| (1,1965) | 1:49:A:LEU:HD21 | 1:219:A:LEU:H | 7 | 0.13 |
| (1,1965) | 1:49:A:LEU:HD22 | 1:219:A:LEU:H | 7 | 0.13 |
| (1,1965) | 1:49:A:LEU:HD23 | 1:219:A:LEU:H | 7 | 0.13 |
| (1,1927) | 1:36:A:GLU:H | 1:36:A:GLU:HG2 | 1 | 0.13 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 16 | 0.13 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 13 | 0.13 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 13 | 0.13 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 13 | 0.13 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 13 | 0.13 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 13 | 0.13 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 13 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD11 | 1:140:A:GLN:H | 6 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD12 | 1:140:A:GLN:H | 6 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD13 | 1:140:A:GLN:H | 6 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD21 | 1:140:A:GLN:H | 6 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD22 | 1:140:A:GLN:H | 6 | 0.13 |
| (1,1808) | 1:3:A:LEU:HD23 | 1:140:A:GLN:H | 6 | 0.13 |
| (1,1782) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HA | 2 | 0.13 |
| (1,1782) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HA | 2 | 0.13 |
| (1,1782) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HA | 2 | 0.13 |
| (1,1771) | 1:67:A:ILE:HG12 | 1:68:A:GLU:HB2 | 12 | 0.13 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 1 | 0.13 |
| (1,1739) | 1:115:A:LYS:HB2 | 1:116:A:GLN:HA | 10 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 9 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 9 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 9 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 11 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 11 | 0.13 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 11 | 0.13 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD11 | 8 | 0.13 |
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD12 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1695) | 1:92:A:THR:HB | 1:93:A:ILE:HD13 | 8 | 0.13 |
| (1,1693) | 1:127:A:GLU:HG2 | 1:130:A:ALA:H | 9 | 0.13 |
| (1,1658) | 1:158:A:VAL:HB | 1:159:A:ASN:H | 17 | 0.13 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 11 | 0.13 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 3 | 0.13 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 16 | 0.13 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 7 | 0.13 |
| (1,1624) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HB2 | 14 | 0.13 |
| (1,1588) | 1:100:A:ALA:HB1 | 1:118:A:LEU:HG | 19 | 0.13 |
| (1,1588) | 1:100:A:ALA:HB2 | 1:118:A:LEU:HG | 19 | 0.13 |
| (1,1588) | 1:100:A:ALA:HB3 | 1:118:A:LEU:HG | 19 | 0.13 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 8 | 0.13 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 8 | 0.13 |
| (1,1577) | 1:164:A:LEU:HD11 | 1:175:A:LEU:HG | 11 | 0.13 |
| (1,1577) | 1:164:A:LEU:HD12 | 1:175:A:LEU:HG | 11 | 0.13 |
| (1,1577) | 1:164:A:LEU:HD13 | 1:175:A:LEU:HG | 11 | 0.13 |
| (1,1577) | 1:164:A:LEU:HD21 | 1:175:A:LEU:HG | 11 | 0.13 |
| (1,1577) | 1:164:A:LEU:HD22 | 1:175:A:LEU:HG | 11 | 0.13 |
| (1,1577) | 1:164:A:LEU:HD23 | 1:175:A:LEU:HG | 11 | 0.13 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 12 | 0.13 |
| (1,1544) | 1:112:A:SER:HA | 1:114:A:LEU:HG | 8 | 0.13 |
| (1,1543) | 1:144:A:ASP:HA | 1:146:A:VAL:H | 7 | 0.13 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB1 | 3 | 0.13 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB2 | 3 | 0.13 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB3 | 3 | 0.13 |
| (1,1524) | 1:118:A:LEU:H | 1:118:A:LEU:HD11 | 12 | 0.13 |
| (1,1524) | 1:118:A:LEU:H | 1:118:A:LEU:HD12 | 12 | 0.13 |
| (1,1524) | 1:118:A:LEU:H | 1:118:A:LEU:HD13 | 12 | 0.13 |
| (1,1521) | 1:172:A:LEU:HD21 | 1:197:A:ALA:HA | 20 | 0.13 |
| (1,1521) | 1:172:A:LEU:HD22 | 1:197:A:ALA:HA | 20 | 0.13 |
| (1,1521) | 1:172:A:LEU:HD23 | 1:197:A:ALA:HA | 20 | 0.13 |
| (1,1500) | 1:130:A:ALA:HB1 | 1:132:A:CYS:H | 10 | 0.13 |
| (1,1500) | 1:130:A:ALA:HB2 | 1:132:A:CYS:H | 10 | 0.13 |
| (1,1500) | 1:130:A:ALA:HB3 | 1:132:A:CYS:H | 10 | 0.13 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 15 | 0.13 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 15 | 0.13 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 15 | 0.13 |
| (1,1483) | 1:34:A:LEU:HD11 | 1:201:A:CYS:HB2 | 3 | 0.13 |
| (1,1483) | 1:34:A:LEU:HD12 | 1:201:A:CYS:HB2 | 3 | 0.13 |
| (1,1483) | 1:34:A:LEU:HD13 | 1:201:A:CYS:HB2 | 3 | 0.13 |
| (1,1483) | 1:34:A:LEU:HD21 | 1:201:A:CYS:HB2 | 3 | 0.13 |
| (1,1483) | 1:34:A:LEU:HD22 | 1:201:A:CYS:HB2 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1483) | 1:34:A:LEU:HD23 | 1:201:A:CYS:HB2 | 3 | 0.13 |
| (1,1415) | 1:86:A:ILE:HG21 | 1:140:A:GLN:HB2 | 2 | 0.13 |
| (1,1415) | 1:86:A:ILE:HG22 | 1:140:A:GLN:HB2 | 2 | 0.13 |
| (1,1415) | 1:86:A:ILE:HG23 | 1:140:A:GLN:HB2 | 2 | 0.13 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB1 | 14 | 0.13 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB2 | 14 | 0.13 |
| (1,1402) | 1:6:A:MET:HA | 1:147:A:ALA:HB3 | 14 | 0.13 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE1 | 3 | 0.13 |
| (1,1386) | 1:92:A:THR:HG21 | 1:133:A:PHE:HE2 | 3 | 0.13 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE1 | 3 | 0.13 |
| (1,1386) | 1:92:A:THR:HG22 | 1:133:A:PHE:HE2 | 3 | 0.13 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE1 | 3 | 0.13 |
| (1,1386) | 1:92:A:THR:HG23 | 1:133:A:PHE:HE2 | 3 | 0.13 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 2 | 0.13 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 11 | 0.13 |
| (1,1306) | 1:48:A:ALA:HB1 | 1:218:A:ALA:HA | 6 | 0.13 |
| (1,1306) | 1:48:A:ALA:HB2 | 1:218:A:ALA:HA | 6 | 0.13 |
| (1,1306) | 1:48:A:ALA:HB3 | 1:218:A:ALA:HA | 6 | 0.13 |
| (1,1262) | 1:156:A:ASP:HA | 1:157:A:LYS:HB2 | 15 | 0.13 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 12 | 0.13 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG11 | 16 | 0.13 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG12 | 16 | 0.13 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG13 | 16 | 0.13 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG21 | 16 | 0.13 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG22 | 16 | 0.13 |
| (1,1216) | 1:215:A:SER:HB2 | 1:217:A:VAL:HG23 | 16 | 0.13 |
| (1,1211) | 1:52:A:LEU:HA | 1:215:A:SER:HB2 | 1 | 0.13 |
| (1,1210) | 1:215:A:SER:HB2 | 1:216:A:ALA:H | 7 | 0.13 |
| (1,1208) | 1:112:A:SER:HB2 | 1:114:A:LEU:HG | 7 | 0.13 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG21 | 11 | 0.13 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG22 | 11 | 0.13 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG23 | 11 | 0.13 |
| (1,1188) | 1:36:A:GLU:H | 1:38:A:SER:HB2 | 12 | 0.13 |
| (1,1187) | 1:32:A:LEU:H | 1:38:A:SER:HB2 | 7 | 0.13 |
| (1,1166) | 1:79:A:VAL:HA | 1:100:A:ALA:HB1 | 11 | 0.13 |
| (1,1166) | 1:79:A:VAL:HA | 1:100:A:ALA:HB2 | 11 | 0.13 |
| (1,1166) | 1:79:A:VAL:HA | 1:100:A:ALA:HB3 | 11 | 0.13 |
| (1,1156) | 1:22:A:VAL:HG11 | 1:108:A:PHE:HA | 15 | 0.13 |
| (1,1156) | 1:22:A:VAL:HG12 | 1:108:A:PHE:HA | 15 | 0.13 |
| (1,1156) | 1:22:A:VAL:HG13 | 1:108:A:PHE:HA | 15 | 0.13 |
| (1,1156) | 1:22:A:VAL:HG21 | 1:108:A:PHE:HA | 15 | 0.13 |
| (1,1156) | 1:22:A:VAL:HG22 | 1:108:A:PHE:HA | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1156) | 1:22:A:VAL:HG23 | 1:108:A:PHE:HA | 15 | 0.13 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 20 | 0.13 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 19 | 0.13 |
| (1,1117) | 1:197:A:ALA:HA | 1:201:A:CYS:HB2 | 1 | 0.13 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 2 | 0.13 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 2 | 0.13 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 2 | 0.13 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 8 | 0.13 |
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 8 | 0.13 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 8 | 0.13 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 14 | 0.13 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 14 | 0.13 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 14 | 0.13 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 20 | 0.13 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 20 | 0.13 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 20 | 0.13 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 18 | 0.13 |
| (1,1043) | 1:192:A:THR:HG21 | 1:193:A:LEU:HA | 3 | 0.13 |
| (1,1043) | 1:192:A:THR:HG22 | 1:193:A:LEU:HA | 3 | 0.13 |
| (1,1043) | 1:192:A:THR:HG23 | 1:193:A:LEU:HA | 3 | 0.13 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 1 | 0.13 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 9 | 0.13 |
| (1,999) | 1:15:A:LYS:H | 1:16:A:VAL:HA | 13 | 0.13 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD21 | 8 | 0.13 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD22 | 8 | 0.13 |
| (1,996) | 1:8:A:ILE:HG12 | 1:52:A:LEU:HD23 | 8 | 0.13 |
| (1,976) | 1:82:A:MET:HE1 | 1:93:A:ILE:H | 17 | 0.13 |
| (1,976) | 1:82:A:MET:HE2 | 1:93:A:ILE:H | 17 | 0.13 |
| (1,976) | 1:82:A:MET:HE3 | 1:93:A:ILE:H | 17 | 0.13 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 10 | 0.13 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB1 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB2 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG11 | 1:147:A:ALA:HB3 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB1 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB2 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG12 | 1:147:A:ALA:HB3 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB1 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB2 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG13 | 1:147:A:ALA:HB3 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB1 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB2 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG21 | 1:147:A:ALA:HB3 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB1 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB2 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG22 | 1:147:A:ALA:HB3 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB1 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB2 | 11 | 0.13 |
| (1,956) | 1:146:A:VAL:HG23 | 1:147:A:ALA:HB3 | 11 | 0.13 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG11 | 20 | 0.13 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG12 | 20 | 0.13 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG13 | 20 | 0.13 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG21 | 20 | 0.13 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG22 | 20 | 0.13 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG23 | 20 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD21 | 2 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD22 | 2 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD23 | 2 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD21 | 6 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD22 | 6 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD23 | 6 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD21 | 18 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD22 | 18 | 0.13 |
| (1,936) | 1:70:A:LEU:HA | 1:70:A:LEU:HD23 | 18 | 0.13 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB1 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB2 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG11 | 1:23:A:ALA:HB3 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB1 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB2 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG12 | 1:23:A:ALA:HB3 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB1 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB2 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG13 | 1:23:A:ALA:HB3 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB1 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB2 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG21 | 1:23:A:ALA:HB3 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB1 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB2 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG22 | 1:23:A:ALA:HB3 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB1 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB2 | 10 | 0.13 |
| (1,926) | 1:22:A:VAL:HG23 | 1:23:A:ALA:HB3 | 10 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD11 | 4 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD12 | 4 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD13 | 4 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD21 | 4 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD22 | 4 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD23 | 4 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD11 | 19 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD12 | 19 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD13 | 19 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD21 | 19 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD22 | 19 | 0.13 |
| (1,920) | 1:193:A:LEU:HA | 1:193:A:LEU:HD23 | 19 | 0.13 |
| (1,886) | 1:217:A:VAL:HB | 1:218:A:ALA:HA | 2 | 0.13 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB1 | 9 | 0.13 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB2 | 9 | 0.13 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB3 | 9 | 0.13 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 7 | 0.13 |
| (1,793) | 1:26:A:TRP:HH2 | 1:46:A:ALA:HA | 15 | 0.13 |
| (1,787) | 1:28:A:PHE:HA | 1:217:A:VAL:HB | 10 | 0.13 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD21 | 19 | 0.13 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD22 | 19 | 0.13 |
| (1,780) | 1:9:A:ASN:H | 1:13:A:LEU:HD23 | 19 | 0.13 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD11 | 18 | 0.13 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD12 | 18 | 0.13 |
| (1,754) | 1:95:A:LEU:H | 1:96:A:ILE:HD13 | 18 | 0.13 |
| (1,731) | 1:194:A:LEU:H | 1:196:A:ASP:H | 7 | 0.13 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 6 | 0.13 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 11 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 9 | 0.13 |
| (1,681) | 1:194:A:LEU:HA | 1:197:A:ALA:H | 8 | 0.13 |
| (1,676) | 1:171:A:HIS:H | 1:171:A:HIS:HD2 | 18 | 0.13 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 1 | 0.13 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 1 | 0.13 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 1 | 0.13 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 3 | 0.13 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 16 | 0.13 |
| (1,632) | 1:34:A:LEU:HD11 | 1:35:A:GLU:H | 7 | 0.13 |
| (1,632) | 1:34:A:LEU:HD12 | 1:35:A:GLU:H | 7 | 0.13 |
| (1,632) | 1:34:A:LEU:HD13 | 1:35:A:GLU:H | 7 | 0.13 |
| (1,632) | 1:34:A:LEU:HD21 | 1:35:A:GLU:H | 7 | 0.13 |
| (1,632) | 1:34:A:LEU:HD22 | 1:35:A:GLU:H | 7 | 0.13 |
| (1,632) | 1:34:A:LEU:HD23 | 1:35:A:GLU:H | 7 | 0.13 |
| (1,630) | 1:112:A:SER:HA | 1:114:A:LEU:H | 16 | 0.13 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 9 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 17 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 17 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 17 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 17 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 17 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 17 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 18 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 18 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 18 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 18 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 18 | 0.13 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 18 | 0.13 |
| (1,548) | 1:112:A:SER:HB2 | 1:114:A:LEU:H | 20 | 0.13 |
| (1,543) | 1:60:A:GLU:H | 1:62:A:PHE:H | 4 | 0.13 |
| (1,512) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 6 | 0.13 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD11 | 5 | 0.13 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD12 | 5 | 0.13 |
| (1,511) | 1:9:A:ASN:H | 1:13:A:LEU:HD13 | 5 | 0.13 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD1 | 4 | 0.13 |
| (1,489) | 1:203:A:GLU:H | 1:204:A:PHE:HD2 | 4 | 0.13 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB1 | 14 | 0.13 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB2 | 14 | 0.13 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB3 | 14 | 0.13 |
| (1,479) | 1:192:A:THR:H | 1:193:A:LEU:HB2 | 8 | 0.13 |
| (1,472) | 1:186:A:GLY:H | 1:187:A:ALA:HB1 | 13 | 0.13 |
| (1,472) | 1:186:A:GLY:H | 1:187:A:ALA:HB2 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,472) | 1:186:A:GLY:H | 1:187:A:ALA:HB3 | 13 | 0.13 |
| (1,457) | 1:152:A:CYS:HA | 1:153:A:ARG:H | 20 | 0.13 |
| (1,427) | 1:212:A:VAL:HG11 | 1:214:A:PHE:H | 20 | 0.13 |
| (1,427) | 1:212:A:VAL:HG12 | 1:214:A:PHE:H | 20 | 0.13 |
| (1,427) | 1:212:A:VAL:HG13 | 1:214:A:PHE:H | 20 | 0.13 |
| (1,427) | 1:212:A:VAL:HG21 | 1:214:A:PHE:H | 20 | 0.13 |
| (1,427) | 1:212:A:VAL:HG22 | 1:214:A:PHE:H | 20 | 0.13 |
| (1,427) | 1:212:A:VAL:HG23 | 1:214:A:PHE:H | 20 | 0.13 |
| (1,416) | 1:193:A:LEU:HD11 | 1:197:A:ALA:H | 4 | 0.13 |
| (1,416) | 1:193:A:LEU:HD12 | 1:197:A:ALA:H | 4 | 0.13 |
| (1,416) | 1:193:A:LEU:HD13 | 1:197:A:ALA:H | 4 | 0.13 |
| (1,416) | 1:193:A:LEU:HD21 | 1:197:A:ALA:H | 4 | 0.13 |
| (1,416) | 1:193:A:LEU:HD22 | 1:197:A:ALA:H | 4 | 0.13 |
| (1,416) | 1:193:A:LEU:HD23 | 1:197:A:ALA:H | 4 | 0.13 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 11 | 0.13 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 11 | 0.13 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 11 | 0.13 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 3 | 0.13 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 14 | 0.13 |
| (1,373) | 1:26:A:TRP:H | 1:106:A:LEU:HG | 16 | 0.13 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 4 | 0.13 |
| (1,364) | 1:17:A:LEU:H | 1:19:A:ARG:HB2 | 8 | 0.13 |
| (1,333) | 1:98:A:ALA:H | 1:100:A:ALA:H | 6 | 0.13 |
| (1,333) | 1:98:A:ALA:H | 1:100:A:ALA:H | 18 | 0.13 |
| (1,317) | 1:206:A:GLU:H | 1:208:A:GLU:H | 12 | 0.13 |
| (1,255) | 1:70:A:LEU:HA | 1:72:A:GLY:H | 13 | 0.13 |
| (1,253) | 1:186:A:GLY:H | 1:187:A:ALA:H | 8 | 0.13 |
| (1,239) | 1:77:A:PRO:HD2 | 1:169:A:ASP:H | 13 | 0.13 |
| (1,229) | 1:213:A:ARG:H | 1:214:A:PHE:HA | 8 | 0.13 |
| (1,217) | 1:26:A:TRP:HB2 | 1:222:A:ALA:H | 17 | 0.13 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 10 | 0.13 |
| (1,179) | 1:213:A:ARG:H | 1:214:A:PHE:HB2 | 7 | 0.13 |
| (1,177) | 1:173:A:TYR:HE1 | 1:184:A:ASN:H | 13 | 0.13 |
| (1,177) | 1:173:A:TYR:HE2 | 1:184:A:ASN:H | 13 | 0.13 |
| (1,165) | 1:155:A:ASP:H | 1:156:A:ASP:HB2 | 14 | 0.13 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 4 | 0.13 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 4 | 0.13 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 4 | 0.13 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 9 | 0.13 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 9 | 0.13 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 9 | 0.13 |
| (1,90) | 1:63:A:ARG:H | 1:64:A:LYS:HG2 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD11 | 11 | 0.13 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD12 | 11 | 0.13 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD13 | 11 | 0.13 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD21 | 11 | 0.13 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD22 | 11 | 0.13 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD23 | 11 | 0.13 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 2 | 0.13 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 5 | 0.13 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 5 | 0.13 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 5 | 0.13 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 5 | 0.13 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 5 | 0.13 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 5 | 0.13 |
| (1,9) | 1:157:A:LYS:H | 1:157:A:LYS:HB2 | 5 | 0.13 |
| (1,8) | 1:156:A:ASP:HB2 | 1:157:A:LYS:H | 14 | 0.13 |
| (1,2370) | 1:221:A:LYS:HB2 | 1:222:A:ALA:HA | 12 | 0.12 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 7 | 0.12 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 19 | 0.12 |
| (1,2322) | 1:184:A:ASN:H | 1:184:A:ASN:HD21 | 12 | 0.12 |
| (1,2322) | 1:184:A:ASN:H | 1:184:A:ASN:HD22 | 12 | 0.12 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 13 | 0.12 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 13 | 0.12 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 13 | 0.12 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 13 | 0.12 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 13 | 0.12 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 13 | 0.12 |
| (1,2300) | 1:172:A:LEU:HD11 | 1:173:A:TYR:HA | 11 | 0.12 |
| (1,2300) | 1:172:A:LEU:HD12 | 1:173:A:TYR:HA | 11 | 0.12 |
| (1,2300) | 1:172:A:LEU:HD13 | 1:173:A:TYR:HA | 11 | 0.12 |
| (1,2300) | 1:172:A:LEU:HD21 | 1:173:A:TYR:HA | 11 | 0.12 |
| (1,2300) | 1:172:A:LEU:HD22 | 1:173:A:TYR:HA | 11 | 0.12 |
| (1,2300) | 1:172:A:LEU:HD23 | 1:173:A:TYR:HA | 11 | 0.12 |
| (1,2292) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HB2 | 4 | 0.12 |
| (1,2292) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HB2 | 4 | 0.12 |
| (1,2292) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HB2 | 4 | 0.12 |
| (1,2292) | 1:168:A:VAL:HG21 | 1:173:A:TYR:HB2 | 4 | 0.12 |
| (1,2292) | 1:168:A:VAL:HG22 | 1:173:A:TYR:HB2 | 4 | 0.12 |
| (1,2292) | 1:168:A:VAL:HG23 | 1:173:A:TYR:HB2 | 4 | 0.12 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 19 | 0.12 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 19 | 0.12 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD11 | 15 | 0.12 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD12 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD13 | 15 | 0.12 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD21 | 15 | 0.12 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD22 | 15 | 0.12 |
| (1,2249) | 1:164:A:LEU:HG | 1:175:A:LEU:HD23 | 15 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD21 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HD22 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD21 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HD22 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD21 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HD22 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD21 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HD22 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD21 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HD22 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD21 | 1 | 0.12 |
| (1,2242) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HD22 | 1 | 0.12 |
| (1,2226) | 1:148:A:GLN:H | 1:148:A:GLN:HG2 | 16 | 0.12 |
| (1,2210) | 1:136:A:ASN:HD21 | 1:137:A:GLU:HB2 | 6 | 0.12 |
| (1,2210) | 1:136:A:ASN:HD22 | 1:137:A:GLU:HB2 | 6 | 0.12 |
| (1,2181) | 1:122:A:GLU:HB2 | 1:123:A:LYS:H | 2 | 0.12 |
| (1,2167) | 1:116:A:GLN:HG2 | 1:119:A:SER:HB2 | 19 | 0.12 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD11 | 6 | 0.12 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD12 | 6 | 0.12 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD13 | 6 | 0.12 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD21 | 6 | 0.12 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD22 | 6 | 0.12 |
| (1,2124) | 1:103:A:GLN:HE22 | 1:118:A:LEU:HD23 | 6 | 0.12 |
| (1,2079) | 1:82:A:MET:HE1 | 1:93:A:ILE:HG12 | 11 | 0.12 |
| (1,2079) | 1:82:A:MET:HE2 | 1:93:A:ILE:HG12 | 11 | 0.12 |
| (1,2079) | 1:82:A:MET:HE3 | 1:93:A:ILE:HG12 | 11 | 0.12 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 12 | 0.12 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 12 | 0.12 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 12 | 0.12 |
| (1,2066) | 1:79:A:VAL:HG11 | 1:173:A:TYR:H | 15 | 0.12 |
| (1,2066) | 1:79:A:VAL:HG12 | 1:173:A:TYR:H | 15 | 0.12 |
| (1,2066) | 1:79:A:VAL:HG13 | 1:173:A:TYR:H | 15 | 0.12 |
| (1,2066) | 1:79:A:VAL:HG21 | 1:173:A:TYR:H | 15 | 0.12 |
| (1,2066) | 1:79:A:VAL:HG22 | 1:173:A:TYR:H | 15 | 0.12 |
| (1,2066) | 1:79:A:VAL:HG23 | 1:173:A:TYR:H | 15 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 4 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 4 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 4 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 4 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 4 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 7 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 7 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 7 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 7 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 7 | 0.12 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 7 | 0.12 |
| (1,2056) | 1:79:A:VAL:HB | 1:168:A:VAL:HG11 | 4 | 0.12 |
| (1,2056) | 1:79:A:VAL:HB | 1:168:A:VAL:HG12 | 4 | 0.12 |
| (1,2056) | 1:79:A:VAL:HB | 1:168:A:VAL:HG13 | 4 | 0.12 |
| (1,2056) | 1:79:A:VAL:HB | 1:168:A:VAL:HG21 | 4 | 0.12 |
| (1,2056) | 1:79:A:VAL:HB | 1:168:A:VAL:HG22 | 4 | 0.12 |
| (1,2056) | 1:79:A:VAL:HB | 1:168:A:VAL:HG23 | 4 | 0.12 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 13 | 0.12 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 13 | 0.12 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 13 | 0.12 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 13 | 0.12 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 13 | 0.12 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 13 | 0.12 |
| (1,2033) | 1:70:A:LEU:HD11 | 1:185:A:HIS:H | 14 | 0.12 |
| (1,2033) | 1:70:A:LEU:HD12 | 1:185:A:HIS:H | 14 | 0.12 |
| (1,2033) | 1:70:A:LEU:HD13 | 1:185:A:HIS:H | 14 | 0.12 |
| (1,2033) | 1:70:A:LEU:HD21 | 1:185:A:HIS:H | 14 | 0.12 |
| (1,2033) | 1:70:A:LEU:HD22 | 1:185:A:HIS:H | 14 | 0.12 |
| (1,2033) | 1:70:A:LEU:HD23 | 1:185:A:HIS:H | 14 | 0.12 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 9 | 0.12 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 9 | 0.12 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 9 | 0.12 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 9 | 0.12 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 9 | 0.12 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 9 | 0.12 |
| (1,2018) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HD2 | 9 | 0.12 |
| (1,2000) | 1:57:A:ALA:HB1 | 1:58:A:GLN:HG2 | 3 | 0.12 |
| (1,2000) | 1:57:A:ALA:HB2 | 1:58:A:GLN:HG2 | 3 | 0.12 |
| (1,2000) | 1:57:A:ALA:HB3 | 1:58:A:GLN:HG2 | 3 | 0.12 |
| (1,1966) | 1:49:A:LEU:HD11 | 1:219:A:LEU:HB2 | 8 | 0.12 |
| (1,1966) | 1:49:A:LEU:HD12 | 1:219:A:LEU:HB2 | 8 | 0.12 |
| (1,1966) | 1:49:A:LEU:HD13 | 1:219:A:LEU:HB2 | 8 | 0.12 |
| (1,1966) | 1:49:A:LEU:HD21 | 1:219:A:LEU:HB2 | 8 | 0.12 |
| (1,1966) | 1:49:A:LEU:HD22 | 1:219:A:LEU:HB2 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1966) | 1:49:A:LEU:HD23 | 1:219:A:LEU:HB2 | 8 | 0.12 |
| (1,1965) | 1:49:A:LEU:HD11 | 1:219:A:LEU:H | 4 | 0.12 |
| (1,1965) | 1:49:A:LEU:HD12 | 1:219:A:LEU:H | 4 | 0.12 |
| (1,1965) | 1:49:A:LEU:HD13 | 1:219:A:LEU:H | 4 | 0.12 |
| (1,1965) | 1:49:A:LEU:HD21 | 1:219:A:LEU:H | 4 | 0.12 |
| (1,1965) | 1:49:A:LEU:HD22 | 1:219:A:LEU:H | 4 | 0.12 |
| (1,1965) | 1:49:A:LEU:HD23 | 1:219:A:LEU:H | 4 | 0.12 |
| (1,1949) | 1:46:A:ALA:HB1 | 1:220:A:CYS:HB2 | 13 | 0.12 |
| (1,1949) | 1:46:A:ALA:HB2 | 1:220:A:CYS:HB2 | 13 | 0.12 |
| (1,1949) | 1:46:A:ALA:HB3 | 1:220:A:CYS:HB2 | 13 | 0.12 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 16 | 0.12 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 19 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD11 | 10 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD12 | 10 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD13 | 10 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD21 | 10 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD22 | 10 | 0.12 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD23 | 10 | 0.12 |
| (1,1932) | 1:36:A:GLU:HG2 | 1:37:A:GLU:H | 19 | 0.12 |
| (1,1923) | 1:33:A:GLY:HA2 | 1:194:A:LEU:HG | 17 | 0.12 |
| (1,1875) | 1:23:A:ALA:H | 1:107:A:GLY:HA2 | 14 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 6 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 6 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 6 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 6 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 6 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 6 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD11 | 1:141:A:ALA:H | 10 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD12 | 1:141:A:ALA:H | 10 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD13 | 1:141:A:ALA:H | 10 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD21 | 1:141:A:ALA:H | 10 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD22 | 1:141:A:ALA:H | 10 | 0.12 |
| (1,1813) | 1:3:A:LEU:HD23 | 1:141:A:ALA:H | 10 | 0.12 |
| (1,1751) | 1:118:A:LEU:HG | 1:121:A:THR:HB | 18 | 0.12 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 16 | 0.12 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 16 | 0.12 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 16 | 0.12 |
| (1,1730) | 1:108:A:PHE:HA | 1:109:A:GLU:HG2 | 17 | 0.12 |
| (1,1724) | 1:74:A:GLU:HG2 | 1:75:A:VAL:H | 19 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 5 | 0.12 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 5 | 0.12 |
| (1,1663) | 1:23:A:ALA:HA | 1:108:A:PHE:HB2 | 2 | 0.12 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG11 | 2 | 0.12 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG12 | 2 | 0.12 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG13 | 2 | 0.12 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG21 | 2 | 0.12 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG22 | 2 | 0.12 |
| (1,1652) | 1:153:A:ARG:HG2 | 1:154:A:VAL:HG23 | 2 | 0.12 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 11 | 0.12 |
| (1,1646) | 1:172:A:LEU:HB2 | 1:187:A:ALA:HA | 9 | 0.12 |
| (1,1634) | 1:77:A:PRO:HB2 | 1:78:A:LYS:HG2 | 20 | 0.12 |
| (1,1629) | 1:131:A:LYS:HA | 1:135:A:LYS:HG2 | 5 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB1 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB2 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB3 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB1 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB2 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB3 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB1 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB2 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB3 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB1 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB2 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB3 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB1 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB2 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB3 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB1 | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB2 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB3 | 9 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB1 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB2 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG11 | 1:218:A:ALA:HB3 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB1 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB2 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG12 | 1:218:A:ALA:HB3 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB1 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB2 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG13 | 1:218:A:ALA:HB3 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB1 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB2 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG21 | 1:218:A:ALA:HB3 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB1 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB2 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG22 | 1:218:A:ALA:HB3 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB1 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB2 | 14 | 0.12 |
| (1,1603) | 1:31:A:VAL:HG23 | 1:218:A:ALA:HB3 | 14 | 0.12 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 9 | 0.12 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 9 | 0.12 |
| (1,1579) | 1:200:A:VAL:HG21 | 1:201:A:CYS:H | 20 | 0.12 |
| (1,1579) | 1:200:A:VAL:HG22 | 1:201:A:CYS:H | 20 | 0.12 |
| (1,1579) | 1:200:A:VAL:HG23 | 1:201:A:CYS:H | 20 | 0.12 |
| (1,1572) | 1:221:A:LYS:HD2 | 1:222:A:ALA:H | 19 | 0.12 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 11 | 0.12 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 13 | 0.12 |
| (1,1563) | 1:212:A:VAL:HB | 1:213:A:ARG:HA | 14 | 0.12 |
| (1,1541) | 1:112:A:SER:HA | 1:113:A:VAL:HB | 2 | 0.12 |
| (1,1500) | 1:130:A:ALA:HB1 | 1:132:A:CYS:H | 20 | 0.12 |
| (1,1500) | 1:130:A:ALA:HB2 | 1:132:A:CYS:H | 20 | 0.12 |
| (1,1500) | 1:130:A:ALA:HB3 | 1:132:A:CYS:H | 20 | 0.12 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE1 | 5 | 0.12 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE2 | 5 | 0.12 |
| (1,1498) | 1:122:A:GLU:H | 1:124:A:MET:HE3 | 5 | 0.12 |
| (1,1481) | 1:121:A:THR:HG21 | 1:124:A:MET:HG2 | 8 | 0.12 |
| (1,1481) | 1:121:A:THR:HG22 | 1:124:A:MET:HG2 | 8 | 0.12 |
| (1,1481) | 1:121:A:THR:HG23 | 1:124:A:MET:HG2 | 8 | 0.12 |
| (1,1466) | 1:19:A:ARG:HD2 | 1:145:A:ALA:H | 18 | 0.12 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 4 | 0.12 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 19 | 0.12 |
| (1,1348) | 1:157:A:LYS:H | 1:157:A:LYS:HD2 | 11 | 0.12 |
| (1,1348) | 1:157:A:LYS:H | 1:157:A:LYS:HD2 | 20 | 0.12 |
| (1,1344) | 1:133:A:PHE:H | 1:135:A:LYS:HD2 | 2 | 0.12 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 19 | 0.12 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 1 | 0.12 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 19 | 0.12 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD21 | 8 | 0.12 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD22 | 8 | 0.12 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD23 | 8 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 4 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD21 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD22 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB1 | 1:219:A:LEU:HD23 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD21 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD22 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB2 | 1:219:A:LEU:HD23 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD21 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD22 | 12 | 0.12 |
| (1,1308) | 1:48:A:ALA:HB3 | 1:219:A:LEU:HD23 | 12 | 0.12 |
| (1,1284) | 1:80:A:TYR:HD1 | 1:100:A:ALA:HA | 6 | 0.12 |
| (1,1284) | 1:80:A:TYR:HD2 | 1:100:A:ALA:HA | 6 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG11 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG12 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG13 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG21 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG22 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD1 | 1:217:A:VAL:HG23 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG11 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG12 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG13 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG21 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG22 | 17 | 0.12 |
| (1,1251) | 1:28:A:PHE:HD2 | 1:217:A:VAL:HG23 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1247) | 1:55:A:LEU:HB2 | 1:161:A:HIS:H | 11 | 0.12 |
| (1,1238) | 1:55:A:LEU:HG | 1:160:A:PHE:HA | 1 | 0.12 |
| (1,1238) | 1:55:A:LEU:HG | 1:160:A:PHE:HA | 11 | 0.12 |
| (1,1218) | 1:131:A:LYS:HB2 | 1:132:A:CYS:HA | 5 | 0.12 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD1 | 7 | 0.12 |
| (1,1206) | 1:201:A:CYS:HA | 1:204:A:PHE:HD2 | 7 | 0.12 |
| (1,1204) | 1:75:A:VAL:HG11 | 1:76:A:SER:HA | 13 | 0.12 |
| (1,1204) | 1:75:A:VAL:HG12 | 1:76:A:SER:HA | 13 | 0.12 |
| (1,1204) | 1:75:A:VAL:HG13 | 1:76:A:SER:HA | 13 | 0.12 |
| (1,1204) | 1:75:A:VAL:HG21 | 1:76:A:SER:HA | 13 | 0.12 |
| (1,1204) | 1:75:A:VAL:HG22 | 1:76:A:SER:HA | 13 | 0.12 |
| (1,1204) | 1:75:A:VAL:HG23 | 1:76:A:SER:HA | 13 | 0.12 |
| (1,1199) | 1:5:A:PRO:HA | 1:88:A:ASN:H | 16 | 0.12 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 1 | 0.12 |
| (1,1169) | 1:16:A:VAL:HA | 1:19:A:ARG:HA | 19 | 0.12 |
| (1,1154) | 1:30:A:ASP:HB2 | 1:217:A:VAL:HA | 17 | 0.12 |
| (1,1137) | 1:72:A:GLY:HA2 | 1:73:A:GLN:HG2 | 18 | 0.12 |
| (1,1133) | 1:118:A:LEU:HA | 1:122:A:GLU:HA | 10 | 0.12 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 20 | 0.12 |
| (1,1081) | 1:27:A:ARG:H | 1:28:A:PHE:HA | 7 | 0.12 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 17 | 0.12 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 17 | 0.12 |
| (1,1076) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 17 | 0.12 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 13 | 0.12 |
| (1,1055) | 1:52:A:LEU:H | 1:214:A:PHE:HA | 7 | 0.12 |
| (1,1047) | 1:102:A:ASN:HB2 | 1:106:A:LEU:HA | 7 | 0.12 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 14 | 0.12 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG21 | 9 | 0.12 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG22 | 9 | 0.12 |
| (1,991) | 1:92:A:THR:HB | 1:96:A:ILE:HG23 | 9 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG11 | 4 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG12 | 4 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG13 | 4 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG21 | 4 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG22 | 4 | 0.12 |
| (1,954) | 1:142:A:ALA:HA | 1:146:A:VAL:HG23 | 4 | 0.12 |
| (1,940) | 1:154:A:VAL:HG11 | 1:155:A:ASP:HA | 18 | 0.12 |
| (1,940) | 1:154:A:VAL:HG12 | 1:155:A:ASP:HA | 18 | 0.12 |
| (1,940) | 1:154:A:VAL:HG13 | 1:155:A:ASP:HA | 18 | 0.12 |
| (1,940) | 1:154:A:VAL:HG21 | 1:155:A:ASP:HA | 18 | 0.12 |
| (1,940) | 1:154:A:VAL:HG22 | 1:155:A:ASP:HA | 18 | 0.12 |
| (1,940) | 1:154:A:VAL:HG23 | 1:155:A:ASP:HA | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|------------------|----------|---------------|
| (1,911) | 1:137:A:GLU:HA | 1:140:A:GLN:H | 4 | 0.12 |
| (1,911) | 1:137:A:GLU:HA | 1:140:A:GLN:H | 14 | 0.12 |
| (1,909) | 1:209:A:GLN:H | 1:209:A:GLN:HG2 | 18 | 0.12 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 6 | 0.12 |
| (1,877) | 1:8:A:ILE:HG12 | 1:53:A:PHE:H | 14 | 0.12 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB1 | 12 | 0.12 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB2 | 12 | 0.12 |
| (1,830) | 1:113:A:VAL:HA | 1:138:A:ALA:HB3 | 12 | 0.12 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB1 | 9 | 0.12 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB2 | 9 | 0.12 |
| (1,782) | 1:16:A:VAL:HA | 1:142:A:ALA:HB3 | 9 | 0.12 |
| (1,745) | 1:55:A:LEU:H | 1:160:A:PHE:HB2 | 11 | 0.12 |
| (1,740) | 1:150:A:GLY:H | 1:151:A:GLN:H | 3 | 0.12 |
| (1,726) | 1:99:A:VAL:HB | 1:100:A:ALA:H | 17 | 0.12 |
| (1,725) | 1:100:A:ALA:H | 1:101:A:ASN:HA | 8 | 0.12 |
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 15 | 0.12 |
| (1,704) | 1:23:A:ALA:HA | 1:25:A:GLN:H | 15 | 0.12 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 12 | 0.12 |
| (1,681) | 1:194:A:LEU:HA | 1:197:A:ALA:H | 2 | 0.12 |
| (1,672) | 1:76:A:SER:H | 1:77:A:PRO:HD2 | 20 | 0.12 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG21 | 7 | 0.12 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG22 | 7 | 0.12 |
| (1,661) | 1:204:A:PHE:H | 1:205:A:THR:HG23 | 7 | 0.12 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 8 | 0.12 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 15 | 0.12 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 19 | 0.12 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 1 | 0.12 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 7 | 0.12 |
| (1,655) | 1:103:A:GLN:H | 1:106:A:LEU:H | 14 | 0.12 |
| (1,634) | 1:32:A:LEU:H | 1:34:A:LEU:H | 5 | 0.12 |
| (1,634) | 1:32:A:LEU:H | 1:34:A:LEU:H | 11 | 0.12 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 2 | 0.12 |
| (1,604) | 1:124:A:MET:H | 1:125:A:SER:H | 9 | 0.12 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 4 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 5 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 5 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 5 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 5 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 5 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 5 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG11 | 6 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG12 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG13 | 6 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG21 | 6 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG22 | 6 | 0.12 |
| (1,554) | 1:145:A:ALA:H | 1:146:A:VAL:HG23 | 6 | 0.12 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 14 | 0.12 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 2 | 0.12 |
| (1,497) | 1:49:A:LEU:HA | 1:217:A:VAL:H | 3 | 0.12 |
| (1,497) | 1:49:A:LEU:HA | 1:217:A:VAL:H | 6 | 0.12 |
| (1,456) | 1:152:A:CYS:HB2 | 1:153:A:ARG:H | 8 | 0.12 |
| (1,443) | 1:135:A:LYS:H | 1:135:A:LYS:HE2 | 4 | 0.12 |
| (1,427) | 1:212:A:VAL:HG11 | 1:214:A:PHE:H | 15 | 0.12 |
| (1,427) | 1:212:A:VAL:HG12 | 1:214:A:PHE:H | 15 | 0.12 |
| (1,427) | 1:212:A:VAL:HG13 | 1:214:A:PHE:H | 15 | 0.12 |
| (1,427) | 1:212:A:VAL:HG21 | 1:214:A:PHE:H | 15 | 0.12 |
| (1,427) | 1:212:A:VAL:HG22 | 1:214:A:PHE:H | 15 | 0.12 |
| (1,427) | 1:212:A:VAL:HG23 | 1:214:A:PHE:H | 15 | 0.12 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG11 | 4 | 0.12 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG12 | 4 | 0.12 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG13 | 4 | 0.12 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG21 | 4 | 0.12 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG22 | 4 | 0.12 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG23 | 4 | 0.12 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 7 | 0.12 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 7 | 0.12 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 7 | 0.12 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 18 | 0.12 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 18 | 0.12 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 18 | 0.12 |
| (1,383) | 1:7:A:GLU:HB2 | 1:8:A:ILE:H | 1 | 0.12 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 20 | 0.12 |
| (1,354) | 1:23:A:ALA:HB1 | 1:25:A:GLN:HE22 | 12 | 0.12 |
| (1,354) | 1:23:A:ALA:HB2 | 1:25:A:GLN:HE22 | 12 | 0.12 |
| (1,354) | 1:23:A:ALA:HB3 | 1:25:A:GLN:HE22 | 12 | 0.12 |
| (1,343) | 1:212:A:VAL:H | 1:213:A:ARG:HB2 | 15 | 0.12 |
| (1,311) | 1:24:A:GLY:H | 1:26:A:TRP:H | 15 | 0.12 |
| (1,253) | 1:186:A:GLY:H | 1:187:A:ALA:H | 2 | 0.12 |
| (1,253) | 1:186:A:GLY:H | 1:187:A:ALA:H | 17 | 0.12 |
| (1,232) | 1:136:A:ASN:HD22 | 1:137:A:GLU:H | 19 | 0.12 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 14 | 0.12 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 14 | 0.12 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 14 | 0.12 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 15 | 0.12 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 15 | 0.12 |
| (1,142) | 1:124:A:MET:H | 1:124:A:MET:HG2 | 20 | 0.12 |
| (1,141) | 1:122:A:GLU:HA | 1:124:A:MET:H | 18 | 0.12 |
| (1,114) | 1:89:A:SER:H | 1:90:A:CYS:H | 16 | 0.12 |
| (1,79) | 1:49:A:LEU:HD11 | 1:50:A:LEU:H | 11 | 0.12 |
| (1,79) | 1:49:A:LEU:HD12 | 1:50:A:LEU:H | 11 | 0.12 |
| (1,79) | 1:49:A:LEU:HD13 | 1:50:A:LEU:H | 11 | 0.12 |
| (1,78) | 1:31:A:VAL:HG11 | 1:50:A:LEU:H | 4 | 0.12 |
| (1,78) | 1:31:A:VAL:HG12 | 1:50:A:LEU:H | 4 | 0.12 |
| (1,78) | 1:31:A:VAL:HG13 | 1:50:A:LEU:H | 4 | 0.12 |
| (1,78) | 1:31:A:VAL:HG21 | 1:50:A:LEU:H | 4 | 0.12 |
| (1,78) | 1:31:A:VAL:HG22 | 1:50:A:LEU:H | 4 | 0.12 |
| (1,78) | 1:31:A:VAL:HG23 | 1:50:A:LEU:H | 4 | 0.12 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD11 | 6 | 0.12 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD12 | 6 | 0.12 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD13 | 6 | 0.12 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD21 | 6 | 0.12 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD22 | 6 | 0.12 |
| (1,74) | 1:48:A:ALA:H | 1:193:A:LEU:HD23 | 6 | 0.12 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 14 | 0.12 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 16 | 0.12 |
| (1,62) | 1:38:A:SER:HA | 1:40:A:GLY:H | 11 | 0.12 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG11 | 19 | 0.12 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG12 | 19 | 0.12 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG13 | 19 | 0.12 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG21 | 19 | 0.12 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG22 | 19 | 0.12 |
| (1,26) | 1:21:A:GLY:H | 1:22:A:VAL:HG23 | 19 | 0.12 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 14 | 0.12 |
| (1,18) | 1:18:A:TYR:HD1 | 1:19:A:ARG:H | 5 | 0.12 |
| (1,18) | 1:18:A:TYR:HD2 | 1:19:A:ARG:H | 5 | 0.12 |
| (1,2362) | 1:219:A:LEU:HD11 | 1:222:A:ALA:H | 9 | 0.11 |
| (1,2362) | 1:219:A:LEU:HD12 | 1:222:A:ALA:H | 9 | 0.11 |
| (1,2362) | 1:219:A:LEU:HD13 | 1:222:A:ALA:H | 9 | 0.11 |
| (1,2362) | 1:219:A:LEU:HD21 | 1:222:A:ALA:H | 9 | 0.11 |
| (1,2362) | 1:219:A:LEU:HD22 | 1:222:A:ALA:H | 9 | 0.11 |
| (1,2362) | 1:219:A:LEU:HD23 | 1:222:A:ALA:H | 9 | 0.11 |
| (1,2348) | 1:203:A:GLU:H | 1:204:A:PHE:HB2 | 11 | 0.11 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG11 | 18 | 0.11 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG12 | 18 | 0.11 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG13 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG21 | 18 | 0.11 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG22 | 18 | 0.11 |
| (1,2339) | 1:199:A:LYS:H | 1:200:A:VAL:HG23 | 18 | 0.11 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD11 | 14 | 0.11 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD12 | 14 | 0.11 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD13 | 14 | 0.11 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 14 | 0.11 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 14 | 0.11 |
| (1,2310) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 14 | 0.11 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD11 | 20 | 0.11 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD12 | 20 | 0.11 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD13 | 20 | 0.11 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD21 | 20 | 0.11 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD22 | 20 | 0.11 |
| (1,2305) | 1:173:A:TYR:HB2 | 1:175:A:LEU:HD23 | 20 | 0.11 |
| (1,2280) | 1:167:A:ASN:HD21 | 1:189:A:SER:H | 15 | 0.11 |
| (1,2280) | 1:167:A:ASN:HD22 | 1:189:A:SER:H | 15 | 0.11 |
| (1,2271) | 1:167:A:ASN:HB2 | 1:170:A:GLY:H | 14 | 0.11 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG11 | 8 | 0.11 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG12 | 8 | 0.11 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG13 | 8 | 0.11 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG21 | 8 | 0.11 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG22 | 8 | 0.11 |
| (1,2268) | 1:167:A:ASN:H | 1:168:A:VAL:HG23 | 8 | 0.11 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE21 | 20 | 0.11 |
| (1,2230) | 1:151:A:GLN:H | 1:151:A:GLN:HE22 | 20 | 0.11 |
| (1,2193) | 1:131:A:LYS:H | 1:132:A:CYS:HB2 | 15 | 0.11 |
| (1,2190) | 1:128:A:ASP:HA | 1:132:A:CYS:HB2 | 1 | 0.11 |
| (1,2141) | 1:108:A:PHE:HA | 1:109:A:GLU:HB2 | 20 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD21 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD22 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD21 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD22 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD21 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD22 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD21 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD22 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD21 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD22 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD21 | 7 | 0.11 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD22 | 7 | 0.11 |
| (1,2079) | 1:82:A:MET:HE1 | 1:93:A:ILE:HG12 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2079) | 1:82:A:MET:HE2 | 1:93:A:ILE:HG12 | 1 | 0.11 |
| (1,2079) | 1:82:A:MET:HE3 | 1:93:A:ILE:HG12 | 1 | 0.11 |
| (1,2067) | 1:79:A:VAL:HG11 | 1:173:A:TYR:HA | 13 | 0.11 |
| (1,2067) | 1:79:A:VAL:HG12 | 1:173:A:TYR:HA | 13 | 0.11 |
| (1,2067) | 1:79:A:VAL:HG13 | 1:173:A:TYR:HA | 13 | 0.11 |
| (1,2067) | 1:79:A:VAL:HG21 | 1:173:A:TYR:HA | 13 | 0.11 |
| (1,2067) | 1:79:A:VAL:HG22 | 1:173:A:TYR:HA | 13 | 0.11 |
| (1,2067) | 1:79:A:VAL:HG23 | 1:173:A:TYR:HA | 13 | 0.11 |
| (1,2065) | 1:79:A:VAL:HG11 | 1:169:A:ASP:H | 11 | 0.11 |
| (1,2065) | 1:79:A:VAL:HG12 | 1:169:A:ASP:H | 11 | 0.11 |
| (1,2065) | 1:79:A:VAL:HG13 | 1:169:A:ASP:H | 11 | 0.11 |
| (1,2065) | 1:79:A:VAL:HG21 | 1:169:A:ASP:H | 11 | 0.11 |
| (1,2065) | 1:79:A:VAL:HG22 | 1:169:A:ASP:H | 11 | 0.11 |
| (1,2065) | 1:79:A:VAL:HG23 | 1:169:A:ASP:H | 11 | 0.11 |
| (1,2063) | 1:79:A:VAL:HG11 | 1:168:A:VAL:HB | 5 | 0.11 |
| (1,2063) | 1:79:A:VAL:HG12 | 1:168:A:VAL:HB | 5 | 0.11 |
| (1,2063) | 1:79:A:VAL:HG13 | 1:168:A:VAL:HB | 5 | 0.11 |
| (1,2063) | 1:79:A:VAL:HG21 | 1:168:A:VAL:HB | 5 | 0.11 |
| (1,2063) | 1:79:A:VAL:HG22 | 1:168:A:VAL:HB | 5 | 0.11 |
| (1,2063) | 1:79:A:VAL:HG23 | 1:168:A:VAL:HB | 5 | 0.11 |
| (1,2059) | 1:79:A:VAL:HG11 | 1:81:A:PHE:HA | 18 | 0.11 |
| (1,2059) | 1:79:A:VAL:HG12 | 1:81:A:PHE:HA | 18 | 0.11 |
| (1,2059) | 1:79:A:VAL:HG13 | 1:81:A:PHE:HA | 18 | 0.11 |
| (1,2059) | 1:79:A:VAL:HG21 | 1:81:A:PHE:HA | 18 | 0.11 |
| (1,2059) | 1:79:A:VAL:HG22 | 1:81:A:PHE:HA | 18 | 0.11 |
| (1,2059) | 1:79:A:VAL:HG23 | 1:81:A:PHE:HA | 18 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG11 | 1:79:A:VAL:HG11 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG11 | 1:79:A:VAL:HG12 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG11 | 1:79:A:VAL:HG13 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG11 | 1:79:A:VAL:HG21 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG11 | 1:79:A:VAL:HG22 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG11 | 1:79:A:VAL:HG23 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG12 | 1:79:A:VAL:HG11 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG12 | 1:79:A:VAL:HG12 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG12 | 1:79:A:VAL:HG13 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG12 | 1:79:A:VAL:HG21 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG12 | 1:79:A:VAL:HG22 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG12 | 1:79:A:VAL:HG23 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG13 | 1:79:A:VAL:HG11 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG13 | 1:79:A:VAL:HG12 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG13 | 1:79:A:VAL:HG13 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG13 | 1:79:A:VAL:HG21 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2040) | 1:75:A:VAL:HG13 | 1:79:A:VAL:HG22 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG13 | 1:79:A:VAL:HG23 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG21 | 1:79:A:VAL:HG11 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG21 | 1:79:A:VAL:HG12 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG21 | 1:79:A:VAL:HG13 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG21 | 1:79:A:VAL:HG21 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG21 | 1:79:A:VAL:HG22 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG21 | 1:79:A:VAL:HG23 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG22 | 1:79:A:VAL:HG11 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG22 | 1:79:A:VAL:HG12 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG22 | 1:79:A:VAL:HG13 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG22 | 1:79:A:VAL:HG21 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG22 | 1:79:A:VAL:HG22 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG22 | 1:79:A:VAL:HG23 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG23 | 1:79:A:VAL:HG11 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG23 | 1:79:A:VAL:HG12 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG23 | 1:79:A:VAL:HG13 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG23 | 1:79:A:VAL:HG21 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG23 | 1:79:A:VAL:HG22 | 6 | 0.11 |
| (1,2040) | 1:75:A:VAL:HG23 | 1:79:A:VAL:HG23 | 6 | 0.11 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 11 | 0.11 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 11 | 0.11 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 11 | 0.11 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 11 | 0.11 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 11 | 0.11 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 11 | 0.11 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD11 | 17 | 0.11 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD12 | 17 | 0.11 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD13 | 17 | 0.11 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD21 | 17 | 0.11 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD22 | 17 | 0.11 |
| (1,2020) | 1:67:A:ILE:HA | 1:70:A:LEU:HD23 | 17 | 0.11 |
| (1,2016) | 1:61:A:ASN:HD21 | 1:62:A:PHE:HB2 | 19 | 0.11 |
| (1,2016) | 1:61:A:ASN:HD22 | 1:62:A:PHE:HB2 | 19 | 0.11 |
| (1,2007) | 1:58:A:GLN:HB2 | 1:59:A:HIS:H | 1 | 0.11 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE21 | 14 | 0.11 |
| (1,2006) | 1:58:A:GLN:HA | 1:58:A:GLN:HE22 | 14 | 0.11 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD11 | 16 | 0.11 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD12 | 16 | 0.11 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD13 | 16 | 0.11 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD21 | 16 | 0.11 |
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD22 | 16 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1955) | 1:49:A:LEU:H | 1:49:A:LEU:HD23 | 16 | 0.11 |
| (1,1948) | 1:46:A:ALA:HA | 1:220:A:CYS:HB2 | 13 | 0.11 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD11 | 6 | 0.11 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD12 | 6 | 0.11 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD13 | 6 | 0.11 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD21 | 6 | 0.11 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD22 | 6 | 0.11 |
| (1,1878) | 1:24:A:GLY:H | 1:106:A:LEU:HD23 | 6 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD11 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD12 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD13 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD21 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD22 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HD23 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD11 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD12 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD13 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD21 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD22 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HD23 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD11 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD12 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD13 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD21 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD22 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HD23 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD11 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD12 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD13 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD21 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD22 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HD23 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD11 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD12 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD13 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD21 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD22 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HD23 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD11 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD12 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD13 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD21 | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD22 | 13 | 0.11 |
| (1,1862) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HD23 | 13 | 0.11 |
| (1,1861) | 1:13:A:LEU:HD11 | 1:95:A:LEU:HG | 19 | 0.11 |
| (1,1861) | 1:13:A:LEU:HD12 | 1:95:A:LEU:HG | 19 | 0.11 |
| (1,1861) | 1:13:A:LEU:HD13 | 1:95:A:LEU:HG | 19 | 0.11 |
| (1,1861) | 1:13:A:LEU:HD21 | 1:95:A:LEU:HG | 19 | 0.11 |
| (1,1861) | 1:13:A:LEU:HD22 | 1:95:A:LEU:HG | 19 | 0.11 |
| (1,1861) | 1:13:A:LEU:HD23 | 1:95:A:LEU:HG | 19 | 0.11 |
| (1,1823) | 1:6:A:MET:HG2 | 1:7:A:GLU:H | 10 | 0.11 |
| (1,1808) | 1:3:A:LEU:HD11 | 1:140:A:GLN:H | 2 | 0.11 |
| (1,1808) | 1:3:A:LEU:HD12 | 1:140:A:GLN:H | 2 | 0.11 |
| (1,1808) | 1:3:A:LEU:HD13 | 1:140:A:GLN:H | 2 | 0.11 |
| (1,1808) | 1:3:A:LEU:HD21 | 1:140:A:GLN:H | 2 | 0.11 |
| (1,1808) | 1:3:A:LEU:HD22 | 1:140:A:GLN:H | 2 | 0.11 |
| (1,1808) | 1:3:A:LEU:HD23 | 1:140:A:GLN:H | 2 | 0.11 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD1 | 3 | 0.11 |
| (1,1790) | 1:79:A:VAL:HB | 1:173:A:TYR:HD2 | 3 | 0.11 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE1 | 11 | 0.11 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE2 | 11 | 0.11 |
| (1,1745) | 1:31:A:VAL:HB | 1:218:A:ALA:H | 1 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 7 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 7 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 7 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 10 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 10 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 10 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 19 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 19 | 0.11 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 19 | 0.11 |
| (1,1721) | 1:225:A:GLU:HG2 | 1:226:A:HIS:H | 13 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD11 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD12 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG11 | 1:106:A:LEU:HD13 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD11 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD12 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG12 | 1:106:A:LEU:HD13 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD11 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD12 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG13 | 1:106:A:LEU:HD13 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD11 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD12 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG21 | 1:106:A:LEU:HD13 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD11 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD12 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG22 | 1:106:A:LEU:HD13 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD11 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD12 | 2 | 0.11 |
| (1,1701) | 1:99:A:VAL:HG23 | 1:106:A:LEU:HD13 | 2 | 0.11 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD11 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD12 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG21 | 1:96:A:ILE:HD13 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD11 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD12 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG22 | 1:96:A:ILE:HD13 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD11 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD12 | 11 | 0.11 |
| (1,1671) | 1:92:A:THR:HG23 | 1:96:A:ILE:HD13 | 11 | 0.11 |
| (1,1658) | 1:158:A:VAL:HB | 1:159:A:ASN:H | 10 | 0.11 |
| (1,1654) | 1:114:A:LEU:HG | 1:115:A:LYS:H | 2 | 0.11 |
| (1,1600) | 1:33:A:GLY:H | 1:218:A:ALA:HB1 | 20 | 0.11 |
| (1,1600) | 1:33:A:GLY:H | 1:218:A:ALA:HB2 | 20 | 0.11 |
| (1,1600) | 1:33:A:GLY:H | 1:218:A:ALA:HB3 | 20 | 0.11 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD1 | 4 | 0.11 |
| (1,1582) | 1:86:A:ILE:HB | 1:133:A:PHE:HD2 | 4 | 0.11 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB1 | 13 | 0.11 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB2 | 13 | 0.11 |
| (1,1567) | 1:221:A:LYS:H | 1:222:A:ALA:HB3 | 13 | 0.11 |
| (1,1549) | 1:112:A:SER:HB2 | 1:114:A:LEU:HA | 3 | 0.11 |
| (1,1536) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD11 | 10 | 0.11 |
| (1,1536) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD12 | 10 | 0.11 |
| (1,1536) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD13 | 10 | 0.11 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB1 | 15 | 0.11 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB2 | 15 | 0.11 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB3 | 15 | 0.11 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB1 | 7 | 0.11 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB2 | 7 | 0.11 |
| (1,1511) | 1:19:A:ARG:HB2 | 1:142:A:ALA:HB3 | 7 | 0.11 |
| (1,1488) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HA | 5 | 0.11 |
| (1,1488) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HA | 18 | 0.11 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 15 | 0.11 |
| (1,1486) | 1:49:A:LEU:HB2 | 1:166:A:ASN:HA | 20 | 0.11 |
| (1,1465) | 1:212:A:VAL:HB | 1:213:A:ARG:HD2 | 12 | 0.11 |
| (1,1450) | 1:3:A:LEU:HD21 | 1:144:A:ASP:H | 12 | 0.11 |
| (1,1450) | 1:3:A:LEU:HD22 | 1:144:A:ASP:H | 12 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1450) | 1:3:A:LEU:HD23 | 1:144:A:ASP:H | 12 | 0.11 |
| (1,1444) | 1:121:A:THR:HA | 1:129:A:ARG:H | 18 | 0.11 |
| (1,1398) | 1:81:A:PHE:H | 1:82:A:MET:HA | 2 | 0.11 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 3 | 0.11 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 8 | 0.11 |
| (1,1384) | 1:71:A:LYS:HG2 | 1:72:A:GLY:HA2 | 16 | 0.11 |
| (1,1366) | 1:117:A:PHE:H | 1:118:A:LEU:HA | 15 | 0.11 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB1 | 2 | 0.11 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB2 | 2 | 0.11 |
| (1,1363) | 1:86:A:ILE:HA | 1:130:A:ALA:HB3 | 2 | 0.11 |
| (1,1358) | 1:14:A:ASN:H | 1:15:A:LYS:HA | 13 | 0.11 |
| (1,1356) | 1:117:A:PHE:HA | 1:119:A:SER:H | 12 | 0.11 |
| (1,1355) | 1:117:A:PHE:HA | 1:120:A:GLU:HB2 | 10 | 0.11 |
| (1,1336) | 1:13:A:LEU:HB2 | 1:95:A:LEU:HA | 7 | 0.11 |
| (1,1330) | 1:58:A:GLN:H | 1:61:A:ASN:HB2 | 20 | 0.11 |
| (1,1327) | 1:82:A:MET:HE1 | 1:83:A:LYS:H | 4 | 0.11 |
| (1,1327) | 1:82:A:MET:HE2 | 1:83:A:LYS:H | 4 | 0.11 |
| (1,1327) | 1:82:A:MET:HE3 | 1:83:A:LYS:H | 4 | 0.11 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD21 | 11 | 0.11 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD22 | 11 | 0.11 |
| (1,1311) | 1:70:A:LEU:HB2 | 1:70:A:LEU:HD23 | 11 | 0.11 |
| (1,1306) | 1:48:A:ALA:HB1 | 1:218:A:ALA:HA | 17 | 0.11 |
| (1,1306) | 1:48:A:ALA:HB2 | 1:218:A:ALA:HA | 17 | 0.11 |
| (1,1306) | 1:48:A:ALA:HB3 | 1:218:A:ALA:HA | 17 | 0.11 |
| (1,1295) | 1:3:A:LEU:HG | 1:4:A:LYS:H | 3 | 0.11 |
| (1,1286) | 1:147:A:ALA:HA | 1:149:A:GLU:H | 3 | 0.11 |
| (1,1282) | 1:67:A:ILE:HG12 | 1:181:A:PHE:HA | 18 | 0.11 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 14 | 0.11 |
| (1,1217) | 1:18:A:TYR:HD1 | 1:22:A:VAL:HA | 12 | 0.11 |
| (1,1217) | 1:18:A:TYR:HD2 | 1:22:A:VAL:HA | 12 | 0.11 |
| (1,1210) | 1:215:A:SER:HB2 | 1:216:A:ALA:H | 20 | 0.11 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG21 | 12 | 0.11 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG22 | 12 | 0.11 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG23 | 12 | 0.11 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE1 | 10 | 0.11 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE2 | 10 | 0.11 |
| (1,1159) | 1:63:A:ARG:HA | 1:179:A:MET:HE3 | 10 | 0.11 |
| (1,1118) | 1:3:A:LEU:H | 1:86:A:ILE:HG21 | 18 | 0.11 |
| (1,1118) | 1:3:A:LEU:H | 1:86:A:ILE:HG22 | 18 | 0.11 |
| (1,1118) | 1:3:A:LEU:H | 1:86:A:ILE:HG23 | 18 | 0.11 |
| (1,1113) | 1:151:A:GLN:HB2 | 1:152:A:CYS:HB2 | 16 | 0.11 |
| (1,1101) | 1:130:A:ALA:HB1 | 1:131:A:LYS:HB2 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1101) | 1:130:A:ALA:HB2 | 1:131:A:LYS:HB2 | 6 | 0.11 |
| (1,1101) | 1:130:A:ALA:HB3 | 1:131:A:LYS:HB2 | 6 | 0.11 |
| (1,1081) | 1:27:A:ARG:H | 1:28:A:PHE:HA | 5 | 0.11 |
| (1,1081) | 1:27:A:ARG:H | 1:28:A:PHE:HA | 17 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 1 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 1 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 1 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 13 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 13 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 13 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 14 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 14 | 0.11 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 14 | 0.11 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 20 | 0.11 |
| (1,1045) | 1:67:A:ILE:HA | 1:70:A:LEU:HB2 | 9 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG11 | 14 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG12 | 14 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG13 | 14 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG21 | 14 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG22 | 14 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG23 | 14 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG11 | 20 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG12 | 20 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG13 | 20 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG21 | 20 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG22 | 20 | 0.11 |
| (1,994) | 1:28:A:PHE:HA | 1:29:A:VAL:HG23 | 20 | 0.11 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE1 | 18 | 0.11 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE2 | 18 | 0.11 |
| (1,963) | 1:120:A:GLU:H | 1:124:A:MET:HE3 | 18 | 0.11 |
| (1,949) | 1:31:A:VAL:HG11 | 1:49:A:LEU:HA | 20 | 0.11 |
| (1,949) | 1:31:A:VAL:HG12 | 1:49:A:LEU:HA | 20 | 0.11 |
| (1,949) | 1:31:A:VAL:HG13 | 1:49:A:LEU:HA | 20 | 0.11 |
| (1,949) | 1:31:A:VAL:HG21 | 1:49:A:LEU:HA | 20 | 0.11 |
| (1,949) | 1:31:A:VAL:HG22 | 1:49:A:LEU:HA | 20 | 0.11 |
| (1,949) | 1:31:A:VAL:HG23 | 1:49:A:LEU:HA | 20 | 0.11 |
| (1,940) | 1:154:A:VAL:HG11 | 1:155:A:ASP:HA | 20 | 0.11 |
| (1,940) | 1:154:A:VAL:HG12 | 1:155:A:ASP:HA | 20 | 0.11 |
| (1,940) | 1:154:A:VAL:HG13 | 1:155:A:ASP:HA | 20 | 0.11 |
| (1,940) | 1:154:A:VAL:HG21 | 1:155:A:ASP:HA | 20 | 0.11 |
| (1,940) | 1:154:A:VAL:HG22 | 1:155:A:ASP:HA | 20 | 0.11 |
| (1,940) | 1:154:A:VAL:HG23 | 1:155:A:ASP:HA | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,939) | 1:98:A:ALA:HA | 1:101:A:ASN:H | 16 | 0.11 |
| (1,937) | 1:142:A:ALA:HA | 1:145:A:ALA:H | 4 | 0.11 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD1 | 20 | 0.11 |
| (1,924) | 1:168:A:VAL:HG11 | 1:173:A:TYR:HD2 | 20 | 0.11 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD1 | 20 | 0.11 |
| (1,924) | 1:168:A:VAL:HG12 | 1:173:A:TYR:HD2 | 20 | 0.11 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD1 | 20 | 0.11 |
| (1,924) | 1:168:A:VAL:HG13 | 1:173:A:TYR:HD2 | 20 | 0.11 |
| (1,879) | 1:8:A:ILE:HG21 | 1:216:A:ALA:H | 8 | 0.11 |
| (1,879) | 1:8:A:ILE:HG22 | 1:216:A:ALA:H | 8 | 0.11 |
| (1,879) | 1:8:A:ILE:HG23 | 1:216:A:ALA:H | 8 | 0.11 |
| (1,826) | 1:100:A:ALA:HA | 1:103:A:GLN:HE21 | 10 | 0.11 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD21 | 10 | 0.11 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD22 | 10 | 0.11 |
| (1,798) | 1:174:A:GLU:HA | 1:175:A:LEU:HD23 | 10 | 0.11 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 5 | 0.11 |
| (1,792) | 1:46:A:ALA:HA | 1:221:A:LYS:H | 7 | 0.11 |
| (1,767) | 1:7:A:GLU:HA | 1:8:A:ILE:HG12 | 7 | 0.11 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 1 | 0.11 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 13 | 0.11 |
| (1,758) | 1:68:A:GLU:H | 1:70:A:LEU:HB2 | 15 | 0.11 |
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 1 | 0.11 |
| (1,703) | 1:58:A:GLN:H | 1:60:A:GLU:H | 2 | 0.11 |
| (1,698) | 1:137:A:GLU:H | 1:140:A:GLN:H | 18 | 0.11 |
| (1,684) | 1:168:A:VAL:HA | 1:171:A:HIS:H | 5 | 0.11 |
| (1,672) | 1:76:A:SER:H | 1:77:A:PRO:HD2 | 8 | 0.11 |
| (1,672) | 1:76:A:SER:H | 1:77:A:PRO:HD2 | 11 | 0.11 |
| (1,672) | 1:76:A:SER:H | 1:77:A:PRO:HD2 | 15 | 0.11 |
| (1,640) | 1:29:A:VAL:H | 1:219:A:LEU:H | 7 | 0.11 |
| (1,632) | 1:34:A:LEU:HD11 | 1:35:A:GLU:H | 17 | 0.11 |
| (1,632) | 1:34:A:LEU:HD12 | 1:35:A:GLU:H | 17 | 0.11 |
| (1,632) | 1:34:A:LEU:HD13 | 1:35:A:GLU:H | 17 | 0.11 |
| (1,632) | 1:34:A:LEU:HD21 | 1:35:A:GLU:H | 17 | 0.11 |
| (1,632) | 1:34:A:LEU:HD22 | 1:35:A:GLU:H | 17 | 0.11 |
| (1,632) | 1:34:A:LEU:HD23 | 1:35:A:GLU:H | 17 | 0.11 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 14 | 0.11 |
| (1,617) | 1:119:A:SER:H | 1:122:A:GLU:H | 17 | 0.11 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 3 | 0.11 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 19 | 0.11 |
| (1,603) | 1:14:A:ASN:H | 1:28:A:PHE:H | 3 | 0.11 |
| (1,561) | 1:26:A:TRP:H | 1:26:A:TRP:HE1 | 5 | 0.11 |
| (1,535) | 1:117:A:PHE:HA | 1:120:A:GLU:H | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 11 | 0.11 |
| (1,529) | 1:61:A:ASN:H | 1:63:A:ARG:H | 16 | 0.11 |
| (1,528) | 1:60:A:GLU:HA | 1:63:A:ARG:H | 5 | 0.11 |
| (1,518) | 1:3:A:LEU:H | 1:87:A:GLY:H | 16 | 0.11 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 15 | 0.11 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB1 | 16 | 0.11 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB2 | 16 | 0.11 |
| (1,482) | 1:196:A:ASP:H | 1:197:A:ALA:HB3 | 16 | 0.11 |
| (1,457) | 1:152:A:CYS:HA | 1:153:A:ARG:H | 13 | 0.11 |
| (1,454) | 1:112:A:SER:H | 1:115:A:LYS:HB2 | 8 | 0.11 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 13 | 0.11 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 13 | 0.11 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 13 | 0.11 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 10 | 0.11 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 10 | 0.11 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 10 | 0.11 |
| (1,382) | 1:120:A:GLU:H | 1:122:A:GLU:H | 19 | 0.11 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 14 | 0.11 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 10 | 0.11 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 10 | 0.11 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 10 | 0.11 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD11 | 17 | 0.11 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD12 | 17 | 0.11 |
| (1,329) | 1:138:A:ALA:H | 1:139:A:ILE:HD13 | 17 | 0.11 |
| (1,307) | 1:93:A:ILE:HA | 1:95:A:LEU:H | 13 | 0.11 |
| (1,290) | 1:81:A:PHE:H | 1:82:A:MET:H | 12 | 0.11 |
| (1,282) | 1:220:A:CYS:HA | 1:222:A:ALA:H | 7 | 0.11 |
| (1,253) | 1:186:A:GLY:H | 1:187:A:ALA:H | 15 | 0.11 |
| (1,247) | 1:166:A:ASN:H | 1:174:A:GLU:HB2 | 9 | 0.11 |
| (1,247) | 1:166:A:ASN:H | 1:174:A:GLU:HB2 | 17 | 0.11 |
| (1,213) | 1:222:A:ALA:H | 1:223:A:ALA:H | 4 | 0.11 |
| (1,161) | 1:150:A:GLY:HA2 | 1:151:A:GLN:H | 13 | 0.11 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB1 | 20 | 0.11 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB2 | 20 | 0.11 |
| (1,158) | 1:144:A:ASP:H | 1:145:A:ALA:HB3 | 20 | 0.11 |
| (1,141) | 1:122:A:GLU:HA | 1:124:A:MET:H | 7 | 0.11 |
| (1,122) | 1:99:A:VAL:HG11 | 1:102:A:ASN:H | 2 | 0.11 |
| (1,122) | 1:99:A:VAL:HG12 | 1:102:A:ASN:H | 2 | 0.11 |
| (1,122) | 1:99:A:VAL:HG13 | 1:102:A:ASN:H | 2 | 0.11 |
| (1,122) | 1:99:A:VAL:HG21 | 1:102:A:ASN:H | 2 | 0.11 |
| (1,122) | 1:99:A:VAL:HG22 | 1:102:A:ASN:H | 2 | 0.11 |
| (1,122) | 1:99:A:VAL:HG23 | 1:102:A:ASN:H | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,107) | 1:139:A:ILE:HG21 | 1:140:A:GLN:H | 16 | 0.11 |
| (1,107) | 1:139:A:ILE:HG22 | 1:140:A:GLN:H | 16 | 0.11 |
| (1,107) | 1:139:A:ILE:HG23 | 1:140:A:GLN:H | 16 | 0.11 |
| (1,82) | 1:55:A:LEU:H | 1:55:A:LEU:HB2 | 15 | 0.11 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 1 | 0.11 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 3 | 0.11 |
| (1,59) | 1:200:A:VAL:HB | 1:201:A:CYS:H | 9 | 0.11 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 1 | 0.11 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 8 | 0.11 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 19 | 0.11 |
| (1,2241) | 1:158:A:VAL:HG11 | 1:159:A:ASN:HB2 | 6 | 0.1 |
| (1,2241) | 1:158:A:VAL:HG12 | 1:159:A:ASN:HB2 | 6 | 0.1 |
| (1,2241) | 1:158:A:VAL:HG13 | 1:159:A:ASN:HB2 | 6 | 0.1 |
| (1,2241) | 1:158:A:VAL:HG21 | 1:159:A:ASN:HB2 | 6 | 0.1 |
| (1,2241) | 1:158:A:VAL:HG22 | 1:159:A:ASN:HB2 | 6 | 0.1 |
| (1,2241) | 1:158:A:VAL:HG23 | 1:159:A:ASN:HB2 | 6 | 0.1 |
| (1,2210) | 1:136:A:ASN:HD21 | 1:137:A:GLU:HB2 | 3 | 0.1 |
| (1,2210) | 1:136:A:ASN:HD22 | 1:137:A:GLU:HB2 | 3 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD21 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG11 | 1:102:A:ASN:HD22 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD21 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG12 | 1:102:A:ASN:HD22 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD21 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG13 | 1:102:A:ASN:HD22 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD21 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG21 | 1:102:A:ASN:HD22 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD21 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG22 | 1:102:A:ASN:HD22 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD21 | 5 | 0.1 |
| (1,2100) | 1:99:A:VAL:HG23 | 1:102:A:ASN:HD22 | 5 | 0.1 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE1 | 9 | 0.1 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE2 | 9 | 0.1 |
| (1,2073) | 1:81:A:PHE:HB2 | 1:82:A:MET:HE3 | 9 | 0.1 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE21 | 12 | 0.1 |
| (1,2036) | 1:73:A:GLN:HA | 1:73:A:GLN:HE22 | 12 | 0.1 |
| (1,2034) | 1:70:A:LEU:HD11 | 1:185:A:HIS:HA | 17 | 0.1 |
| (1,2034) | 1:70:A:LEU:HD12 | 1:185:A:HIS:HA | 17 | 0.1 |
| (1,2034) | 1:70:A:LEU:HD13 | 1:185:A:HIS:HA | 17 | 0.1 |
| (1,2034) | 1:70:A:LEU:HD21 | 1:185:A:HIS:HA | 17 | 0.1 |
| (1,2034) | 1:70:A:LEU:HD22 | 1:185:A:HIS:HA | 17 | 0.1 |
| (1,2034) | 1:70:A:LEU:HD23 | 1:185:A:HIS:HA | 17 | 0.1 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD11 | 13 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD12 | 13 | 0.1 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD13 | 13 | 0.1 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD21 | 13 | 0.1 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD22 | 13 | 0.1 |
| (1,2025) | 1:70:A:LEU:H | 1:70:A:LEU:HD23 | 13 | 0.1 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD11 | 18 | 0.1 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD12 | 18 | 0.1 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD13 | 18 | 0.1 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD21 | 18 | 0.1 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD22 | 18 | 0.1 |
| (1,1935) | 1:38:A:SER:HB2 | 1:39:A:LEU:HD23 | 18 | 0.1 |
| (1,1903) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 13 | 0.1 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE1 | 1 | 0.1 |
| (1,1786) | 1:18:A:TYR:HA | 1:18:A:TYR:HE2 | 1 | 0.1 |
| (1,1735) | 1:44:A:ALA:HB1 | 1:45:A:PRO:HB2 | 13 | 0.1 |
| (1,1735) | 1:44:A:ALA:HB2 | 1:45:A:PRO:HB2 | 13 | 0.1 |
| (1,1735) | 1:44:A:ALA:HB3 | 1:45:A:PRO:HB2 | 13 | 0.1 |
| (1,1647) | 1:172:A:LEU:HB2 | 1:197:A:ALA:HA | 16 | 0.1 |
| (1,1577) | 1:164:A:LEU:HD11 | 1:175:A:LEU:HG | 2 | 0.1 |
| (1,1577) | 1:164:A:LEU:HD12 | 1:175:A:LEU:HG | 2 | 0.1 |
| (1,1577) | 1:164:A:LEU:HD13 | 1:175:A:LEU:HG | 2 | 0.1 |
| (1,1577) | 1:164:A:LEU:HD21 | 1:175:A:LEU:HG | 2 | 0.1 |
| (1,1577) | 1:164:A:LEU:HD22 | 1:175:A:LEU:HG | 2 | 0.1 |
| (1,1577) | 1:164:A:LEU:HD23 | 1:175:A:LEU:HG | 2 | 0.1 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB1 | 18 | 0.1 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB2 | 18 | 0.1 |
| (1,1532) | 1:142:A:ALA:HA | 1:145:A:ALA:HB3 | 18 | 0.1 |
| (1,1438) | 1:29:A:VAL:HG11 | 1:219:A:LEU:HA | 2 | 0.1 |
| (1,1438) | 1:29:A:VAL:HG12 | 1:219:A:LEU:HA | 2 | 0.1 |
| (1,1438) | 1:29:A:VAL:HG13 | 1:219:A:LEU:HA | 2 | 0.1 |
| (1,1438) | 1:29:A:VAL:HG21 | 1:219:A:LEU:HA | 2 | 0.1 |
| (1,1438) | 1:29:A:VAL:HG22 | 1:219:A:LEU:HA | 2 | 0.1 |
| (1,1438) | 1:29:A:VAL:HG23 | 1:219:A:LEU:HA | 2 | 0.1 |
| (1,1400) | 1:6:A:MET:HA | 1:7:A:GLU:HA | 20 | 0.1 |
| (1,1350) | 1:156:A:ASP:HB2 | 1:158:A:VAL:HA | 5 | 0.1 |
| (1,1350) | 1:156:A:ASP:HB2 | 1:158:A:VAL:HA | 15 | 0.1 |
| (1,1279) | 1:93:A:ILE:HA | 1:164:A:LEU:HD11 | 5 | 0.1 |
| (1,1279) | 1:93:A:ILE:HA | 1:164:A:LEU:HD12 | 5 | 0.1 |
| (1,1279) | 1:93:A:ILE:HA | 1:164:A:LEU:HD13 | 5 | 0.1 |
| (1,1279) | 1:93:A:ILE:HA | 1:164:A:LEU:HD21 | 5 | 0.1 |
| (1,1279) | 1:93:A:ILE:HA | 1:164:A:LEU:HD22 | 5 | 0.1 |
| (1,1279) | 1:93:A:ILE:HA | 1:164:A:LEU:HD23 | 5 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1262) | 1:156:A:ASP:HA | 1:157:A:LYS:HB2 | 8 | 0.1 |
| (1,1259) | 1:58:A:GLN:HA | 1:61:A:ASN:HB2 | 1 | 0.1 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD11 | 17 | 0.1 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD12 | 17 | 0.1 |
| (1,1225) | 1:163:A:ILE:H | 1:163:A:ILE:HD13 | 17 | 0.1 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG21 | 6 | 0.1 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG22 | 6 | 0.1 |
| (1,1207) | 1:201:A:CYS:HA | 1:205:A:THR:HG23 | 6 | 0.1 |
| (1,1154) | 1:30:A:ASP:HB2 | 1:217:A:VAL:HA | 16 | 0.1 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 9 | 0.1 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 9 | 0.1 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 9 | 0.1 |
| (1,1064) | 1:145:A:ALA:HB1 | 1:146:A:VAL:HA | 11 | 0.1 |
| (1,1064) | 1:145:A:ALA:HB2 | 1:146:A:VAL:HA | 11 | 0.1 |
| (1,1064) | 1:145:A:ALA:HB3 | 1:146:A:VAL:HA | 11 | 0.1 |
| (1,1061) | 1:65:A:LYS:H | 1:67:A:ILE:HG12 | 14 | 0.1 |
| (1,1059) | 1:209:A:GLN:HA | 1:209:A:GLN:HG2 | 8 | 0.1 |
| (1,1042) | 1:192:A:THR:HG21 | 1:193:A:LEU:H | 16 | 0.1 |
| (1,1042) | 1:192:A:THR:HG22 | 1:193:A:LEU:H | 16 | 0.1 |
| (1,1042) | 1:192:A:THR:HG23 | 1:193:A:LEU:H | 16 | 0.1 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 15 | 0.1 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 18 | 0.1 |
| (1,1004) | 1:137:A:GLU:HB2 | 1:138:A:ALA:HA | 19 | 0.1 |
| (1,719) | 1:64:A:LYS:H | 1:66:A:GLN:H | 16 | 0.1 |
| (1,656) | 1:103:A:GLN:H | 1:104:A:ASP:HB2 | 17 | 0.1 |
| (1,642) | 1:53:A:PHE:H | 1:160:A:PHE:HB2 | 12 | 0.1 |
| (1,634) | 1:32:A:LEU:H | 1:34:A:LEU:H | 13 | 0.1 |
| (1,632) | 1:34:A:LEU:HD11 | 1:35:A:GLU:H | 13 | 0.1 |
| (1,632) | 1:34:A:LEU:HD12 | 1:35:A:GLU:H | 13 | 0.1 |
| (1,632) | 1:34:A:LEU:HD13 | 1:35:A:GLU:H | 13 | 0.1 |
| (1,632) | 1:34:A:LEU:HD21 | 1:35:A:GLU:H | 13 | 0.1 |
| (1,632) | 1:34:A:LEU:HD22 | 1:35:A:GLU:H | 13 | 0.1 |
| (1,632) | 1:34:A:LEU:HD23 | 1:35:A:GLU:H | 13 | 0.1 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG11 | 13 | 0.1 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG12 | 13 | 0.1 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG13 | 13 | 0.1 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG21 | 13 | 0.1 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG22 | 13 | 0.1 |
| (1,628) | 1:144:A:ASP:H | 1:146:A:VAL:HG23 | 13 | 0.1 |
| (1,611) | 1:95:A:LEU:HG | 1:96:A:ILE:H | 4 | 0.1 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE1 | 1 | 0.1 |
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE2 | 1 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,594) | 1:176:A:ASP:H | 1:179:A:MET:HE3 | 1 | 0.1 |
| (1,590) | 1:123:A:LYS:H | 1:123:A:LYS:HE2 | 5 | 0.1 |
| (1,520) | 1:17:A:LEU:H | 1:19:A:ARG:H | 7 | 0.1 |
| (1,517) | 1:206:A:GLU:H | 1:207:A:ARG:HB2 | 14 | 0.1 |
| (1,426) | 1:213:A:ARG:HA | 1:214:A:PHE:H | 5 | 0.1 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG11 | 1 | 0.1 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG12 | 1 | 0.1 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG13 | 1 | 0.1 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG21 | 1 | 0.1 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG22 | 1 | 0.1 |
| (1,418) | 1:216:A:ALA:H | 1:217:A:VAL:HG23 | 1 | 0.1 |
| (1,404) | 1:100:A:ALA:HB1 | 1:103:A:GLN:HE21 | 8 | 0.1 |
| (1,404) | 1:100:A:ALA:HB2 | 1:103:A:GLN:HE21 | 8 | 0.1 |
| (1,404) | 1:100:A:ALA:HB3 | 1:103:A:GLN:HE21 | 8 | 0.1 |
| (1,402) | 1:98:A:ALA:HB1 | 1:101:A:ASN:H | 6 | 0.1 |
| (1,402) | 1:98:A:ALA:HB2 | 1:101:A:ASN:H | 6 | 0.1 |
| (1,402) | 1:98:A:ALA:HB3 | 1:101:A:ASN:H | 6 | 0.1 |
| (1,369) | 1:143:A:HIS:H | 1:145:A:ALA:H | 5 | 0.1 |
| (1,333) | 1:98:A:ALA:H | 1:100:A:ALA:H | 8 | 0.1 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 17 | 0.1 |
| (1,69) | 1:47:A:CYS:H | 1:48:A:ALA:H | 18 | 0.1 |
| (1,32) | 1:23:A:ALA:H | 1:108:A:PHE:HA | 16 | 0.1 |
| (1,20) | 1:18:A:TYR:HB2 | 1:20:A:LEU:H | 6 | 0.1 |

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

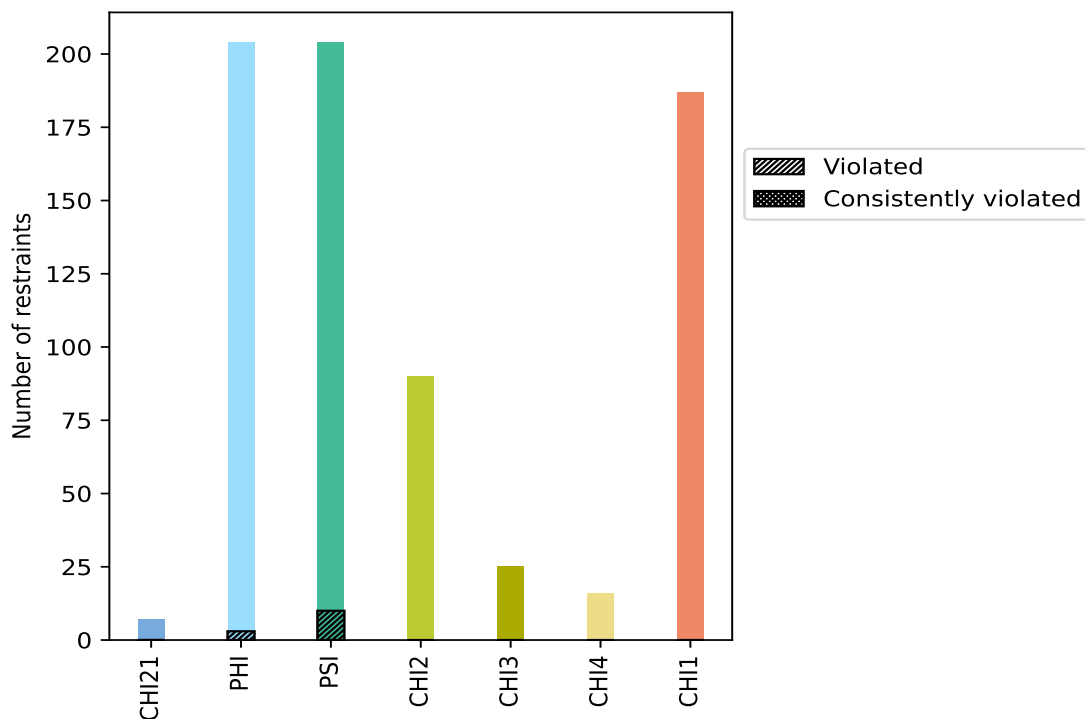
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| CHI21 | 7 | 1.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| PHI | 204 | 27.8 | 3 | 1.5 | 0.4 | 0 | 0.0 | 0.0 |
| PSI | 204 | 27.8 | 10 | 4.9 | 1.4 | 0 | 0.0 | 0.0 |
| CHI2 | 90 | 12.3 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| CHI3 | 25 | 3.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| CHI4 | 16 | 2.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| CHI1 | 187 | 25.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 733 | 100.0 | 13 | 1.8 | 1.8 | 0 | 0.0 | 0.0 |

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

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



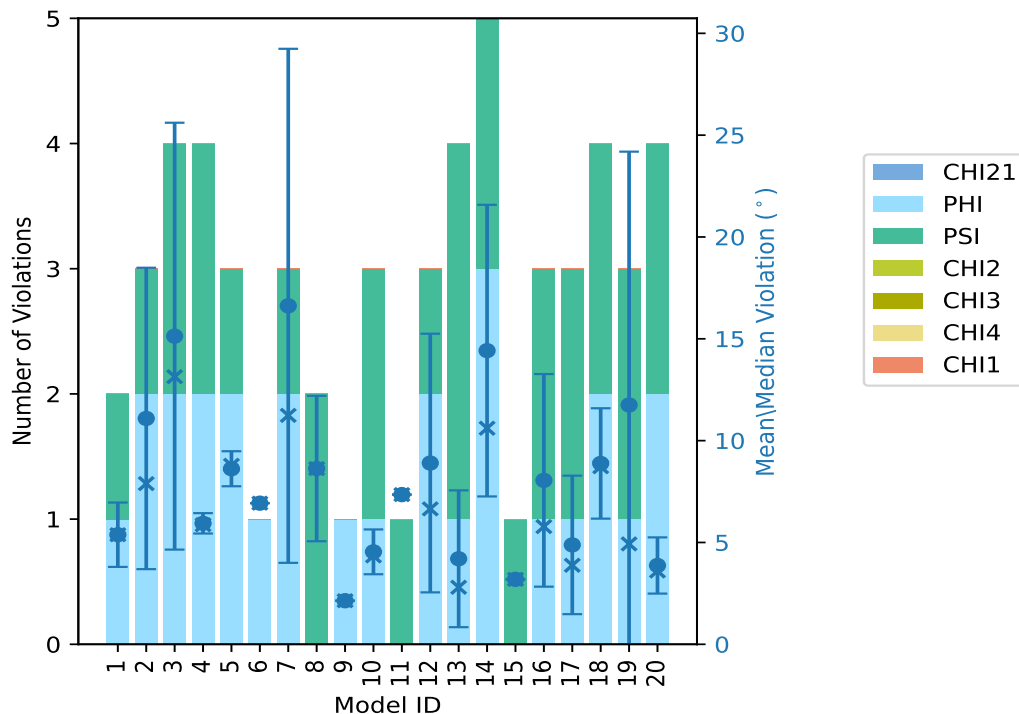
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations | | | | | | | Total | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-----|------|------|------|------|-------|----------|---------|--------|------------|
| | CHI21 | PHI | PSI | CHI2 | CHI3 | CHI4 | CHI1 | | | | | |
| 1 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 2 | 5.38 | 6.97 | 1.58 | 5.38 |
| 2 | 0 | 2 | 1 | 0 | 0 | 0 | 0 | 3 | 11.09 | 21.32 | 7.4 | 7.89 |
| 3 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 4 | 15.13 | 29.22 | 10.48 | 13.14 |
| 4 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 4 | 5.94 | 6.69 | 0.5 | 5.87 |
| 5 | 0 | 2 | 1 | 0 | 0 | 0 | 0 | 3 | 8.62 | 9.57 | 0.86 | 8.79 |
| 6 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 6.93 | 6.93 | 0.0 | 6.93 |
| 7 | 0 | 2 | 1 | 0 | 0 | 0 | 0 | 3 | 16.62 | 34.04 | 12.62 | 11.24 |
| 8 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 2 | 8.63 | 12.2 | 3.57 | 8.63 |
| 9 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 2.14 | 2.14 | 0.0 | 2.14 |
| 10 | 0 | 1 | 2 | 0 | 0 | 0 | 0 | 3 | 4.54 | 5.98 | 1.1 | 4.34 |
| 11 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 7.35 | 7.35 | 0.0 | 7.35 |
| 12 | 0 | 2 | 1 | 0 | 0 | 0 | 0 | 3 | 8.9 | 17.55 | 6.35 | 6.65 |
| 13 | 0 | 1 | 3 | 0 | 0 | 0 | 0 | 4 | 4.2 | 9.9 | 3.36 | 2.8 |
| 14 | 0 | 3 | 2 | 0 | 0 | 0 | 0 | 5 | 14.42 | 27.16 | 7.16 | 10.61 |
| 15 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 3.19 | 3.19 | 0.0 | 3.19 |
| 16 | 0 | 1 | 2 | 0 | 0 | 0 | 0 | 3 | 8.05 | 15.27 | 5.22 | 5.78 |
| 17 | 0 | 1 | 2 | 0 | 0 | 0 | 0 | 3 | 4.88 | 9.45 | 3.4 | 3.88 |
| 18 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 4 | 8.88 | 12.69 | 2.71 | 8.72 |
| 19 | 0 | 1 | 2 | 0 | 0 | 0 | 0 | 3 | 11.75 | 29.21 | 12.44 | 4.93 |
| 20 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 4 | 3.87 | 5.85 | 1.38 | 3.6 |

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



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

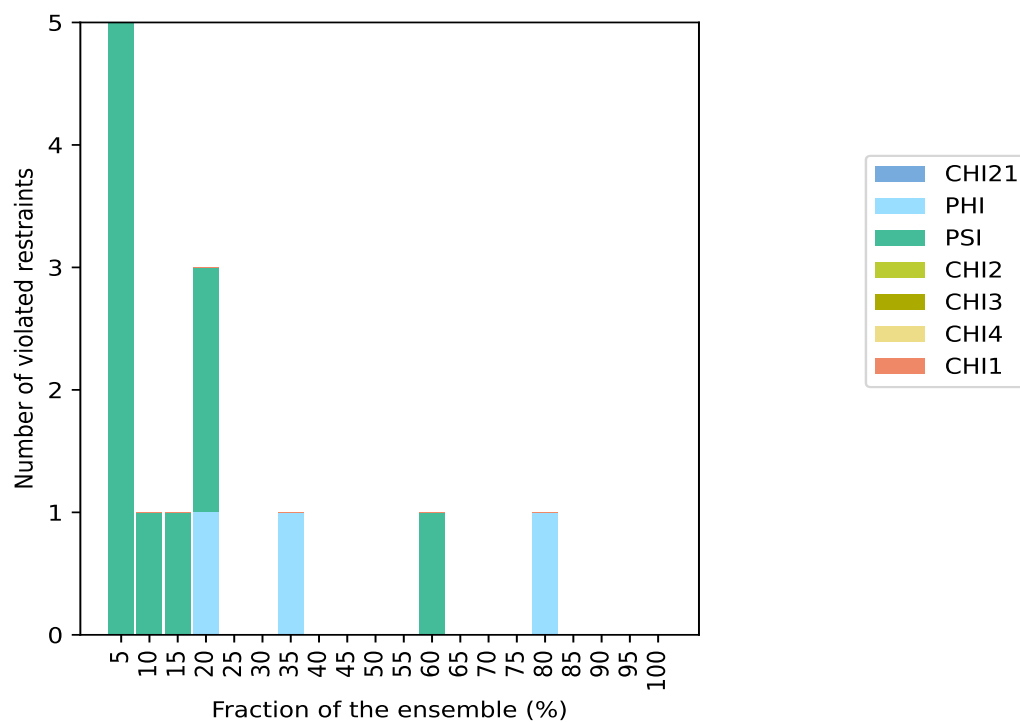
10.3 Dihedral-angle violation statistics for the ensemble

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

| Number of violated restraints | | | | | | | | Fraction of the ensemble | |
|-------------------------------|-----|-----|------|------|------|------|-------|--------------------------|-------|
| CHI21 | PHI | PSI | CHI2 | CHI3 | CHI4 | CHI1 | Total | Count ¹ | % |
| 0 | 0 | 5 | 0 | 0 | 0 | 0 | 5 | 1 | 5.0 |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 2 | 10.0 |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 3 | 15.0 |
| 0 | 1 | 2 | 0 | 0 | 0 | 0 | 3 | 4 | 20.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 25.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 30.0 |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 7 | 35.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | 40.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | 45.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | 50.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | 55.0 |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 12 | 60.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 14 | 70.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 75.0 |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 16 | 80.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 17 | 85.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 18 | 90.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 19 | 95.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 100.0 |

¹ Number of models with violations

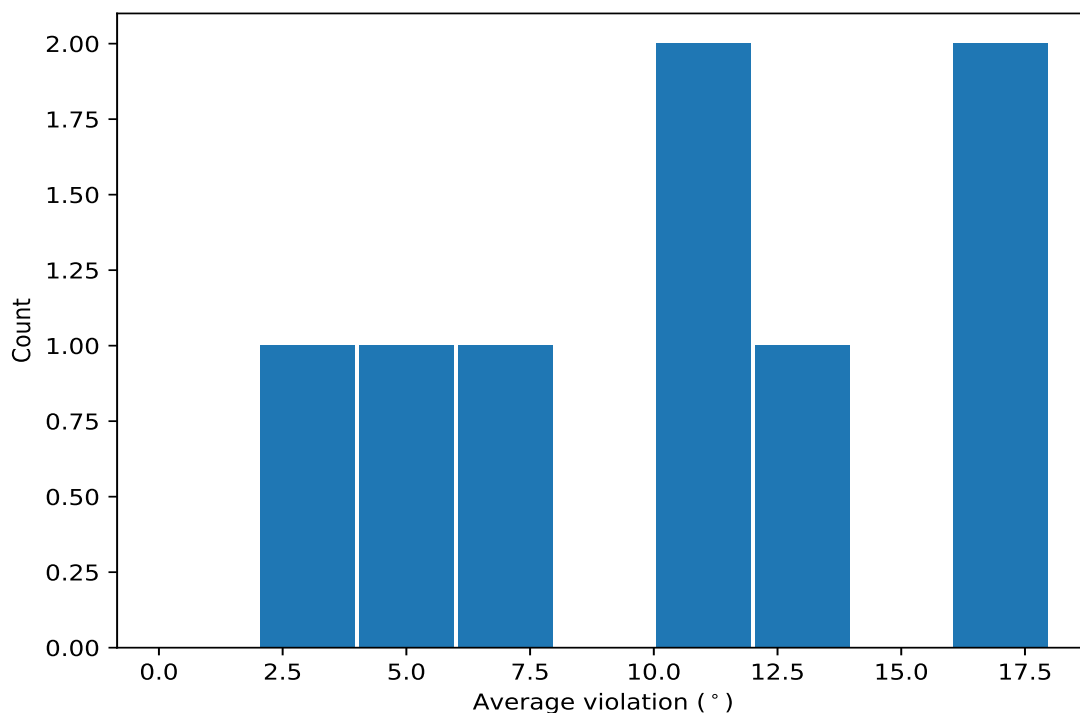
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

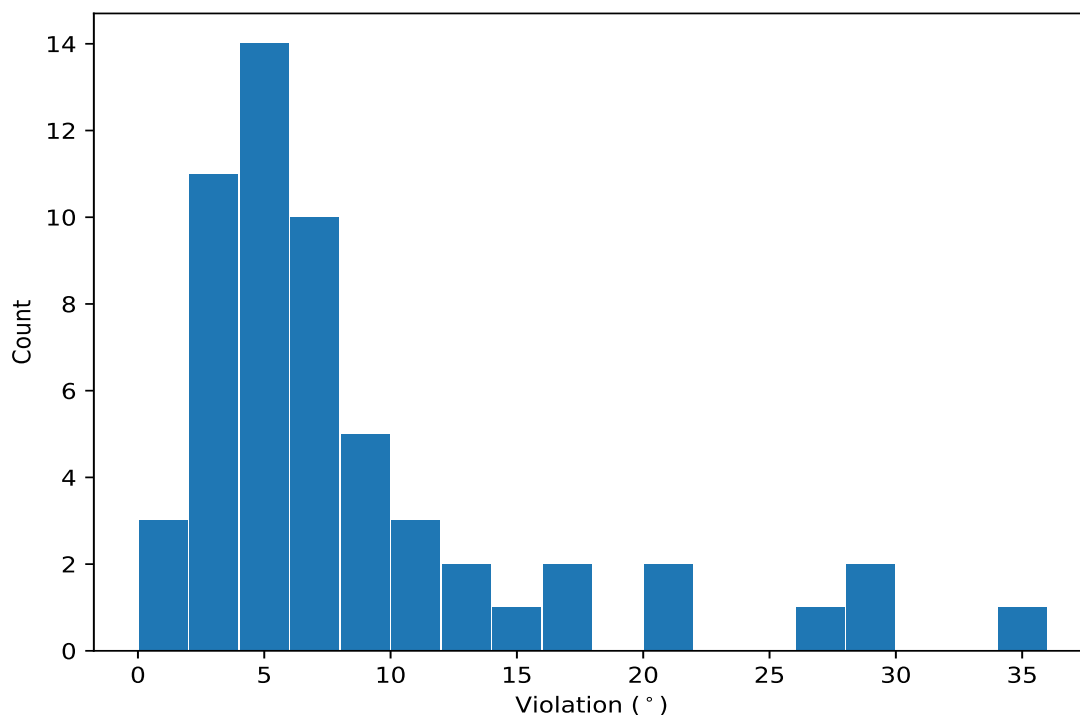
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 16 | 5.59 | 2.24 | 5.46 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 12 | 6.82 | 2.26 | 6.32 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 7 | 16.38 | 8.35 | 15.27 |
| (1,355) | 1:124:A:MET:N | 1:124:A:MET:CA | 1:124:A:MET:C | 1:125:A:SER:N | 4 | 17.4 | 10.42 | 14.88 |
| (1,381) | 1:188:A:SER:N | 1:188:A:SER:CA | 1:188:A:SER:C | 1:189:A:SER:N | 4 | 12.42 | 10.43 | 9.59 |
| (1,249) | 1:178:A:ARG:C | 1:179:A:MET:N | 1:179:A:MET:CA | 1:179:A:MET:C | 4 | 10.0 | 7.1 | 8.13 |
| (1,339) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLN:N | 3 | 2.3 | 0.75 | 2.48 |
| (1,395) | 1:222:A:ALA:N | 1:222:A:ALA:CA | 1:222:A:ALA:C | 1:223:A:ALA:N | 2 | 11.99 | 9.24 | 11.99 |

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

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

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

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



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,355) | 1:124:A:MET:N | 1:124:A:MET:CA | 1:124:A:MET:C | 1:125:A:SER:N | 7 | 34.04 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 3 | 29.22 |
| (1,381) | 1:188:A:SER:N | 1:188:A:SER:CA | 1:188:A:SER:C | 1:189:A:SER:N | 19 | 29.21 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 14 | 27.16 |
| (1,249) | 1:178:A:ARG:C | 1:179:A:MET:N | 1:179:A:MET:CA | 1:179:A:MET:C | 2 | 21.32 |
| (1,395) | 1:222:A:ALA:N | 1:222:A:ALA:CA | 1:222:A:ALA:C | 1:223:A:ALA:N | 3 | 21.23 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 12 | 17.55 |
| (1,355) | 1:124:A:MET:N | 1:124:A:MET:CA | 1:124:A:MET:C | 1:125:A:SER:N | 14 | 17.07 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 16 | 15.27 |
| (1,355) | 1:124:A:MET:N | 1:124:A:MET:CA | 1:124:A:MET:C | 1:125:A:SER:N | 18 | 12.69 |
| (1,381) | 1:188:A:SER:N | 1:188:A:SER:CA | 1:188:A:SER:C | 1:189:A:SER:N | 8 | 12.2 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 7 | 11.24 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 14 | 10.61 |
| (1,249) | 1:178:A:ARG:C | 1:179:A:MET:N | 1:179:A:MET:CA | 1:179:A:MET:C | 14 | 10.26 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 13 | 9.9 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 18 | 9.89 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 5 | 9.57 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 17 | 9.45 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 5 | 8.79 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 2 | 7.89 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 18 | 7.55 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 5 | 7.49 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 11 | 7.35 |
| (1,381) | 1:188:A:SER:N | 1:188:A:SER:CA | 1:188:A:SER:C | 1:189:A:SER:N | 14 | 6.99 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1 | 6.97 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 6 | 6.93 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 4 | 6.69 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 12 | 6.65 |
| (1,249) | 1:178:A:ARG:C | 1:179:A:MET:N | 1:179:A:MET:CA | 1:179:A:MET:C | 4 | 6.0 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 10 | 5.98 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 20 | 5.85 |
| (1,355) | 1:124:A:MET:N | 1:124:A:MET:CA | 1:124:A:MET:C | 1:125:A:SER:N | 16 | 5.78 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 4 | 5.74 |
| (1,103) | 1:75:A:VAL:C | 1:76:A:SER:N | 1:76:A:SER:CA | 1:76:A:SER:C | 18 | 5.4 |
| (1,4) | 1:6:A:MET:N | 1:6:A:MET:CA | 1:6:A:MET:C | 1:7:A:GLU:N | 4 | 5.31 |
| (1,391) | 1:212:A:VAL:N | 1:212:A:VAL:CA | 1:212:A:VAL:C | 1:213:A:ARG:N | 8 | 5.06 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 3 | 5.06 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 3 | 5.01 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 19 | 4.93 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 7 | 4.57 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 20 | 4.46 |
| (1,311) | 1:1:A:MET:N | 1:1:A:MET:CA | 1:1:A:MET:C | 1:2:A:GLN:N | 10 | 4.34 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 2 | 4.06 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 17 | 3.88 |
| (1,52) | 1:42:A:VAL:N | 1:42:A:VAL:CA | 1:42:A:VAL:C | 1:43:A:PRO:N | 1 | 3.8 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 10 | 3.31 |
| (1,112) | 1:81:A:PHE:N | 1:81:A:PHE:CA | 1:81:A:PHE:C | 1:82:A:MET:N | 15 | 3.19 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 13 | 3.12 |
| (1,339) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLN:N | 16 | 3.11 |
| (1,395) | 1:222:A:ALA:N | 1:222:A:ALA:CA | 1:222:A:ALA:C | 1:223:A:ALA:N | 20 | 2.75 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 12 | 2.49 |
| (1,339) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLN:N | 13 | 2.48 |
| (1,249) | 1:178:A:ARG:C | 1:179:A:MET:N | 1:179:A:MET:CA | 1:179:A:MET:C | 20 | 2.41 |
| (1,53) | 1:43:A:PRO:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 9 | 2.14 |
| (1,339) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLN:N | 17 | 1.31 |
| (1,381) | 1:188:A:SER:N | 1:188:A:SER:CA | 1:188:A:SER:C | 1:189:A:SER:N | 13 | 1.29 |
| (1,385) | 1:208:A:GLU:N | 1:208:A:GLU:CA | 1:208:A:GLU:C | 1:209:A:GLN:N | 19 | 1.11 |