



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 11:16 PM EST

PDB ID : 2MR7
BMRB ID : 25064
Title : apo structure of the Peptidyl Carrier Protein Domain 7 of the teicoplanin producing Non-ribosomal peptide synthetase
Authors : Haslinger, K.; Maximowitsch, E.; Redfield, C.; Cryle, M.J.
Deposited on : 2014-07-02

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

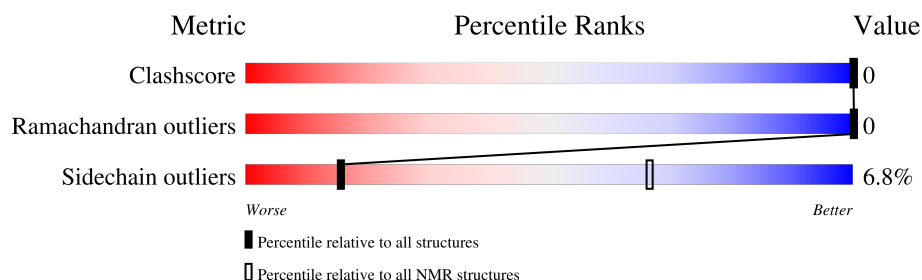
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 73%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 91 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:11-A:77 (67) | 0.39 | 9 |

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1360 atoms, of which 685 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-ribosomal peptide synthetase.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 91 | Total | C | H | N | O | S | 0 |
| | | | 1360 | 426 | 685 | 120 | 126 | 3 | |

There are 13 discrepancies between the modelled and reference sequences:

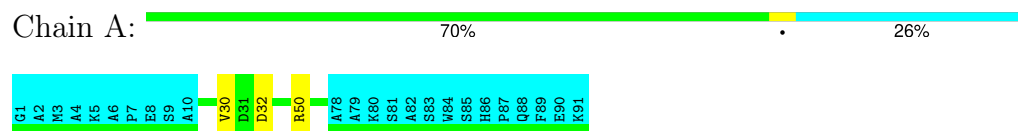
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1 | GLY | - | expression tag | UNP Q70AZ6 |
| A | 2 | ALA | - | expression tag | UNP Q70AZ6 |
| A | 3 | MET | - | expression tag | UNP Q70AZ6 |
| A | 82 | ALA | - | expression tag | UNP Q70AZ6 |
| A | 83 | SER | - | expression tag | UNP Q70AZ6 |
| A | 84 | TRP | - | expression tag | UNP Q70AZ6 |
| A | 85 | SER | - | expression tag | UNP Q70AZ6 |
| A | 86 | HIS | - | expression tag | UNP Q70AZ6 |
| A | 87 | PRO | - | expression tag | UNP Q70AZ6 |
| A | 88 | GLN | - | expression tag | UNP Q70AZ6 |
| A | 89 | PHE | - | expression tag | UNP Q70AZ6 |
| A | 90 | GLU | - | expression tag | UNP Q70AZ6 |
| A | 91 | LYS | - | expression tag | UNP Q70AZ6 |

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: Non-ribosomal peptide synthetase

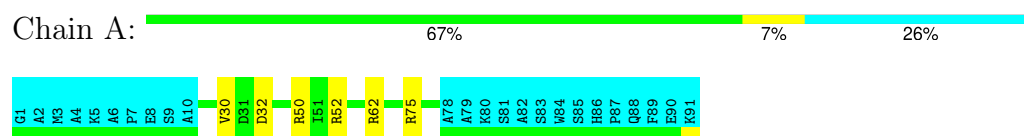


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

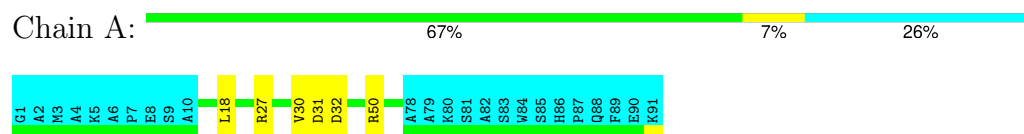
4.2.1 Score per residue for model 1

- Molecule 1: Non-ribosomal peptide synthetase



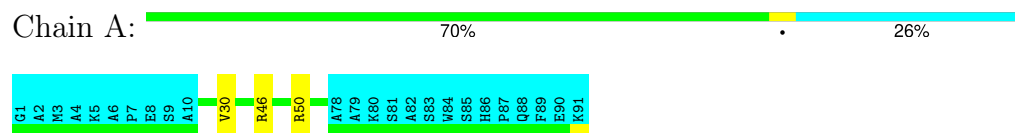
4.2.2 Score per residue for model 2

- Molecule 1: Non-ribosomal peptide synthetase



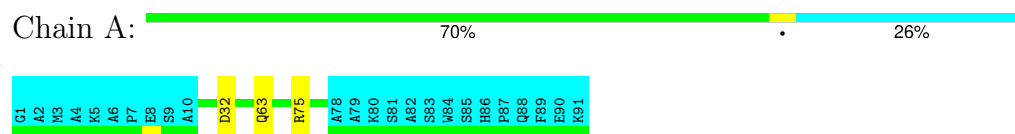
4.2.3 Score per residue for model 3

- Molecule 1: Non-ribosomal peptide synthetase



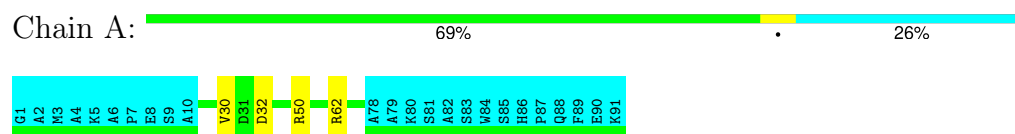
4.2.4 Score per residue for model 4

- Molecule 1: Non-ribosomal peptide synthetase



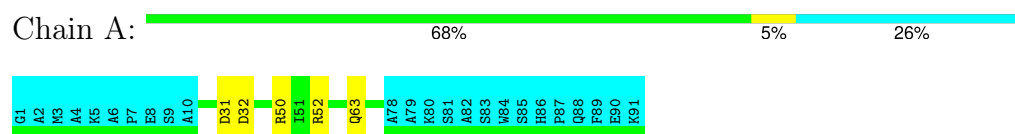
4.2.5 Score per residue for model 5

- Molecule 1: Non-ribosomal peptide synthetase



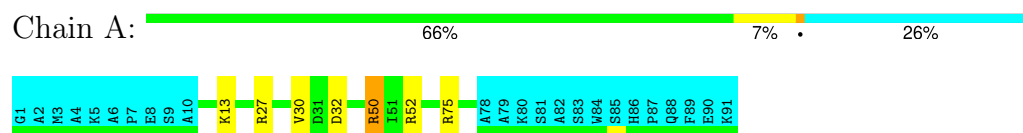
4.2.6 Score per residue for model 6

- Molecule 1: Non-ribosomal peptide synthetase



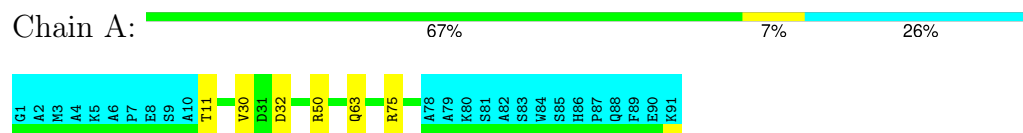
4.2.7 Score per residue for model 7

- Molecule 1: Non-ribosomal peptide synthetase



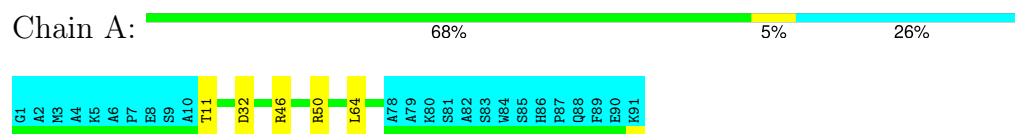
4.2.8 Score per residue for model 8

- Molecule 1: Non-ribosomal peptide synthetase



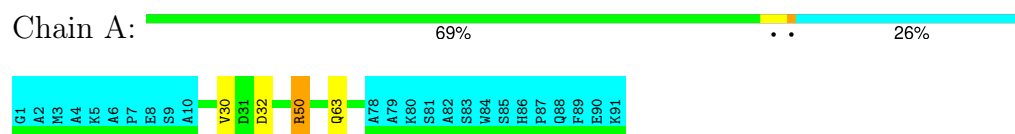
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Non-ribosomal peptide synthetase



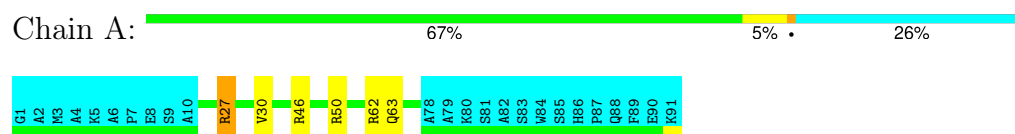
4.2.10 Score per residue for model 10

- Molecule 1: Non-ribosomal peptide synthetase



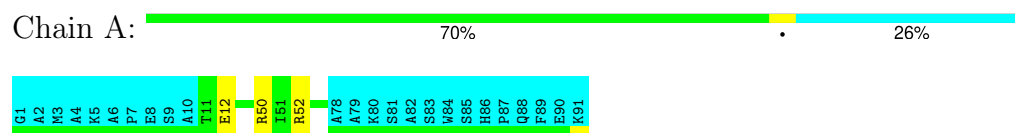
4.2.11 Score per residue for model 11

- Molecule 1: Non-ribosomal peptide synthetase



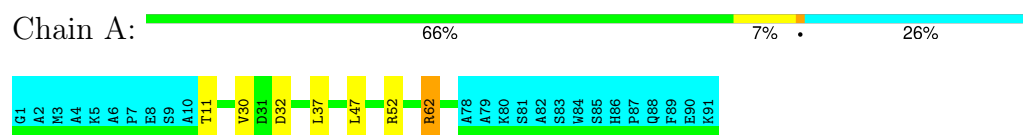
4.2.12 Score per residue for model 12

- Molecule 1: Non-ribosomal peptide synthetase



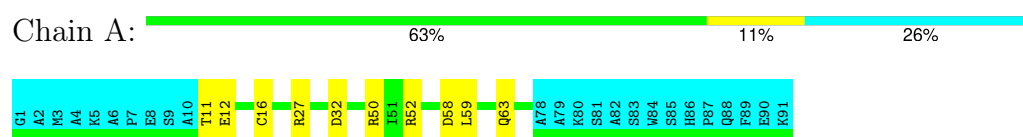
4.2.13 Score per residue for model 13

- Molecule 1: Non-ribosomal peptide synthetase



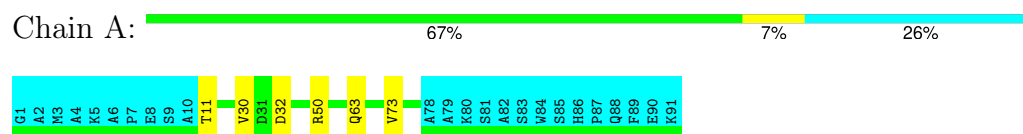
4.2.14 Score per residue for model 14

- Molecule 1: Non-ribosomal peptide synthetase



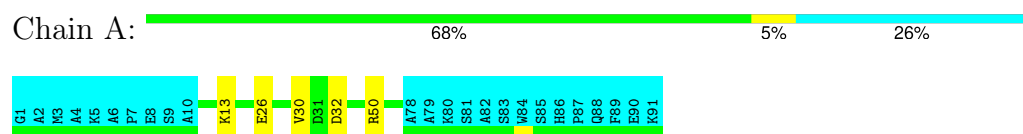
4.2.15 Score per residue for model 15

- Molecule 1: Non-ribosomal peptide synthetase



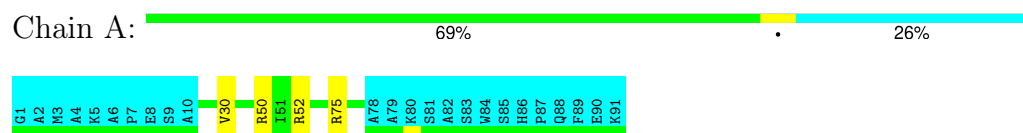
4.2.16 Score per residue for model 16

- Molecule 1: Non-ribosomal peptide synthetase



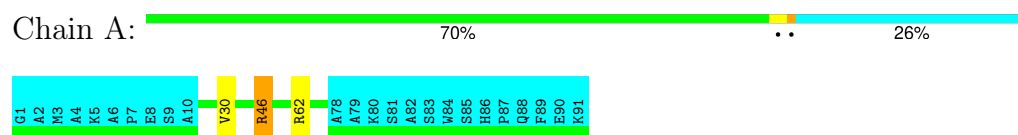
4.2.17 Score per residue for model 17

- Molecule 1: Non-ribosomal peptide synthetase



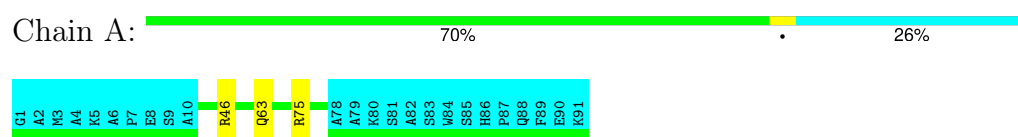
4.2.18 Score per residue for model 18

- Molecule 1: Non-ribosomal peptide synthetase



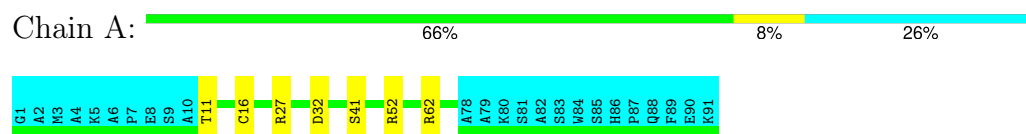
4.2.19 Score per residue for model 19

- Molecule 1: Non-ribosomal peptide synthetase



4.2.20 Score per residue for model 20

- Molecule 1: Non-ribosomal peptide synthetase



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| YASARA | refinement | 2 |
| YASARA | refinement | 2 |
| YASARA | refinement | 2 |
| YASARA | refinement | 2 |
| CYANA | structure solution | |

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 | 4 |
| Total number of shifts | 1986 |
| Number of shifts mapped to atoms | 1986 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 73% |

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 | 0.76±0.07 | 0±0/508 (0.0± 0.0%) | 0.85±0.05 | 2±1/689 (0.3± 0.2%) |
| All | All | 0.77 | 0/10160 (0.0%) | 0.85 | 43/13780 (0.3%) |

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 | 52 | ARG | NE-CZ-NH1 | 7.85 | 124.22 | 120.30 | 20 | 8 |
| 1 | A | 50 | ARG | NE-CZ-NH1 | 7.57 | 124.08 | 120.30 | 16 | 12 |
| 1 | A | 52 | ARG | NE-CZ-NH2 | -6.59 | 117.00 | 120.30 | 7 | 2 |
| 1 | A | 75 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 | 17 | 6 |
| 1 | A | 27 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 | 20 | 3 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 5.59 | 123.10 | 120.30 | 19 | 3 |
| 1 | A | 62 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 | 5 | 5 |
| 1 | A | 50 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 | 10 | 2 |
| 1 | A | 62 | ARG | NE-CZ-NH2 | -5.07 | 117.76 | 120.30 | 20 | 1 |
| 1 | A | 27 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 | 11 | 1 |

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All | 10020 | 10380 | 10380 | - |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1 | A | 67/91 (74%) | 65±1 (97±1%) | 2±1 (3±1%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 1340/1820 (74%) | 1303 (97%) | 37 (3%) | 0 (0%) | 100 | 100 |

There are no Ramachandran outliers.

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 | 52/68 (76%) | 48±2 (93±3%) | 4±2 (7±3%) | 16 | 66 |
| All | All | 1040/1360 (76%) | 969 (93%) | 71 (7%) | 16 | 66 |

All 21 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 | 32 | ASP | 14 |
| 1 | A | 30 | VAL | 13 |
| 1 | A | 63 | GLN | 8 |
| 1 | A | 11 | THR | 6 |
| 1 | A | 50 | ARG | 5 |
| 1 | A | 27 | ARG | 3 |
| 1 | A | 46 | ARG | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 31 | ASP | 2 |
| 1 | A | 13 | LYS | 2 |
| 1 | A | 12 | GLU | 2 |
| 1 | A | 62 | ARG | 2 |
| 1 | A | 16 | CYS | 2 |
| 1 | A | 18 | LEU | 1 |
| 1 | A | 64 | LEU | 1 |
| 1 | A | 37 | LEU | 1 |
| 1 | A | 47 | LEU | 1 |
| 1 | A | 58 | ASP | 1 |
| 1 | A | 59 | LEU | 1 |
| 1 | A | 73 | VAL | 1 |
| 1 | A | 26 | GLU | 1 |
| 1 | A | 41 | SER | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

| | |
|---|-----|
| Total number of shifts | 406 |
| Number of shifts mapped to atoms | 406 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 6 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 47 | LEU | HD11 | 0.755 | 0.001 | 2 |
| 1 | A | 47 | LEU | HD12 | 0.755 | 0.001 | 2 |
| 1 | A | 47 | LEU | HD13 | 0.755 | 0.001 | 2 |
| 1 | A | 37 | LEU | HD11 | 0.917 | . | 2 |
| 1 | A | 37 | LEU | HD12 | 0.917 | . | 2 |
| 1 | A | 37 | LEU | HD13 | 0.917 | . | 2 |

7.1.2 Chemical shift referencing

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

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 37%, i.e. 336 atoms were assigned a chemical shift out of a possible 907. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 58/335 (17%) | 58/137 (42%) | 0/134 (0%) | 0/64 (0%) |
| Sidechain | 262/536 (49%) | 262/354 (74%) | 0/162 (0%) | 0/20 (0%) |
| Aromatic | 16/36 (44%) | 16/18 (89%) | 0/17 (0%) | 0/1 (0%) |
| Overall | 336/907 (37%) | 336/509 (66%) | 0/313 (0%) | 0/85 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 34%, i.e. 400 atoms were assigned a chemical shift out of a possible 1193. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 70/452 (15%) | 70/184 (38%) | 0/182 (0%) | 0/86 (0%) |
| Sidechain | 304/676 (45%) | 304/446 (68%) | 0/206 (0%) | 0/24 (0%) |
| Aromatic | 26/65 (40%) | 26/33 (79%) | 0/29 (0%) | 0/3 (0%) |
| Overall | 400/1193 (34%) | 400/663 (60%) | 0/417 (0%) | 0/113 (0%) |

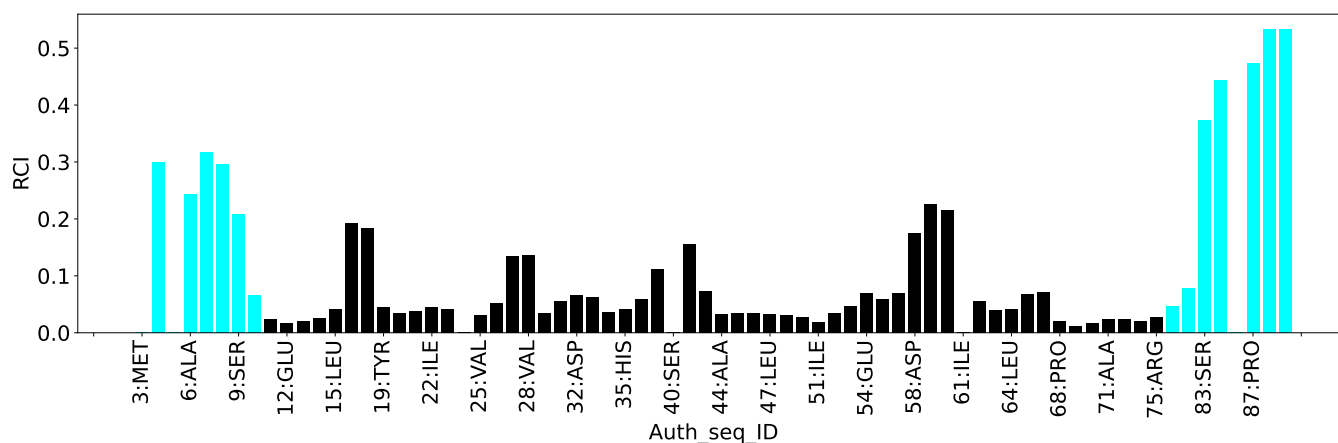
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping ⓘ

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

| | |
|---|-----|
| Total number of shifts | 607 |
| Number of shifts mapped to atoms | 607 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 7 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 2 | A | 47 | LEU | HD11 | 0.746 | 0.007 | 2 |
| 2 | A | 47 | LEU | HD12 | 0.746 | 0.007 | 2 |
| 2 | A | 47 | LEU | HD13 | 0.746 | 0.007 | 2 |
| 2 | A | 37 | LEU | HD11 | 0.923 | . | 1 |
| 2 | A | 37 | LEU | HD12 | 0.923 | . | 1 |
| 2 | A | 37 | LEU | HD13 | 0.923 | . | 1 |
| 2 | A | 77 | LEU | HD11 | 0.815 | . | 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 |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 40 | -0.37 ± 0.19 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 56 | 0.04 ± 0.08 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 0 | — | None (insufficient data) |

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 59%, i.e. 539 atoms were assigned a chemical shift out of a possible 907. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 144/335 (43%) | 109/137 (80%) | 35/134 (26%) | 0/64 (0%) |
| Sidechain | 391/536 (73%) | 286/354 (81%) | 105/162 (65%) | 0/20 (0%) |
| Aromatic | 4/36 (11%) | 4/18 (22%) | 0/17 (0%) | 0/1 (0%) |
| Overall | 539/907 (59%) | 399/509 (78%) | 140/313 (45%) | 0/85 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 600 atoms were assigned a chemical shift out of a possible 1193. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone | 163/452 (36%) | 123/184 (67%) | 40/182 (22%) | 0/86 (0%) |
| Sidechain | 430/676 (64%) | 314/446 (70%) | 116/206 (56%) | 0/24 (0%) |
| Aromatic | 7/65 (11%) | 7/33 (21%) | 0/29 (0%) | 0/3 (0%) |
| Overall | 600/1193 (50%) | 444/663 (67%) | 156/417 (37%) | 0/113 (0%) |

7.2.4 Statistically unusual chemical shifts [i](#)

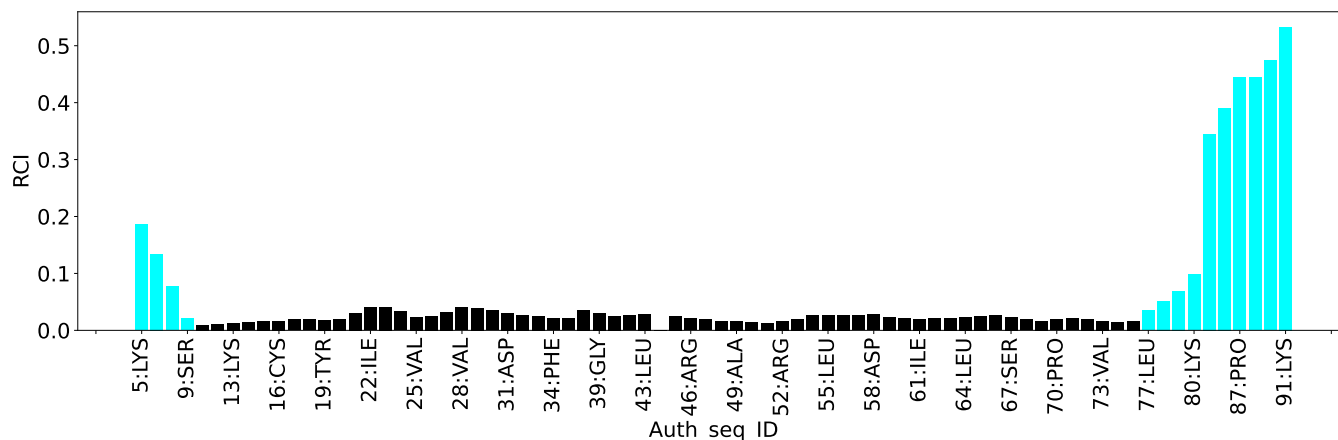
There are no statistically unusual chemical shifts.

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:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 Bookkeeping ⓘ

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

| | |
|---|-----|
| Total number of shifts | 424 |
| Number of shifts mapped to atoms | 424 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 3 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 3 | A | 47 | LEU | HD11 | 0.798 | . | 2 |
| 3 | A | 47 | LEU | HD12 | 0.798 | . | 2 |
| 3 | A | 47 | LEU | HD13 | 0.798 | . | 2 |

7.3.2 Chemical shift referencing [i](#)

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

7.3.3 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 43%, i.e. 387 atoms were assigned a chemical shift out of a possible 907. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 109/335 (33%) | 109/137 (80%) | 0/134 (0%) | 0/64 (0%) |
| Sidechain | 263/536 (49%) | 263/354 (74%) | 0/162 (0%) | 0/20 (0%) |
| Aromatic | 15/36 (42%) | 15/18 (83%) | 0/17 (0%) | 0/1 (0%) |
| Overall | 387/907 (43%) | 387/509 (76%) | 0/313 (0%) | 0/85 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 421 atoms were assigned a chemical shift out of a possible 1193. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 122/452 (27%) | 122/184 (66%) | 0/182 (0%) | 0/86 (0%) |
| Sidechain | 277/676 (41%) | 277/446 (62%) | 0/206 (0%) | 0/24 (0%) |
| Aromatic | 22/65 (34%) | 22/33 (67%) | 0/29 (0%) | 0/3 (0%) |
| Overall | 421/1193 (35%) | 421/663 (63%) | 0/417 (0%) | 0/113 (0%) |

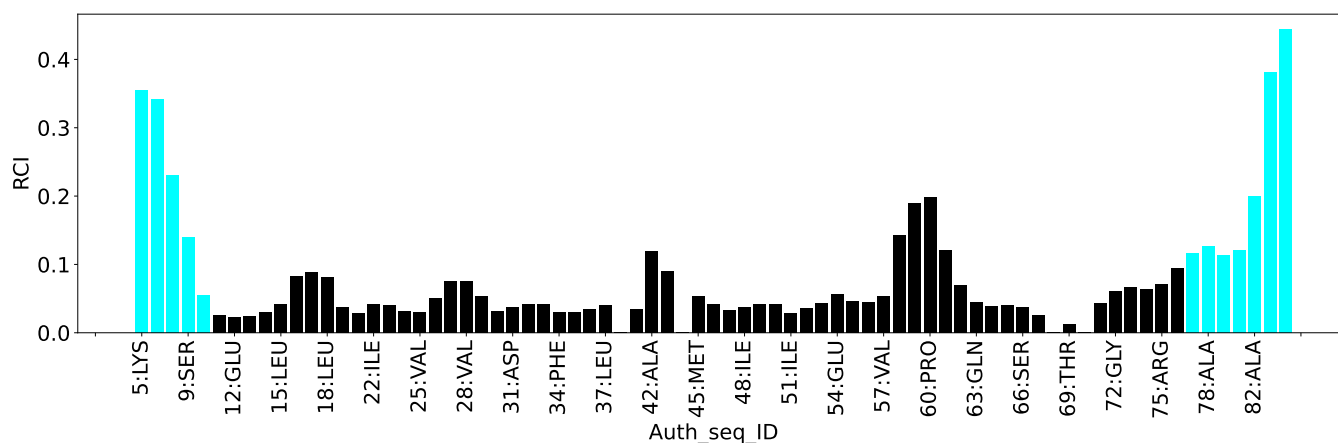
7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.3.5 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:



7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_4*

7.4.1 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 | 549 |
| Number of shifts mapped to atoms | 549 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 6 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 4 | A | 47 | LEU | HD11 | 0.763 | . | 2 |
| 4 | A | 47 | LEU | HD12 | 0.763 | . | 2 |
| 4 | A | 47 | LEU | HD13 | 0.763 | . | 2 |
| 4 | A | 37 | LEU | HD11 | 0.902 | . | 2 |
| 4 | A | 37 | LEU | HD12 | 0.902 | . | 2 |
| 4 | A | 37 | LEU | HD13 | 0.902 | . | 2 |

7.4.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}_\beta$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 69 | 0.12 ± 0.53 | None needed (< 0.5 ppm) |

7.4.3 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 54%, i.e. 494 atoms were assigned a chemical shift out of a possible 907. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 191/335 (57%) | 131/137 (96%) | 0/134 (0%) | 60/64 (94%) |
| Sidechain | 296/536 (55%) | 295/354 (83%) | 0/162 (0%) | 1/20 (5%) |
| Aromatic | 7/36 (19%) | 7/18 (39%) | 0/17 (0%) | 0/1 (0%) |
| Overall | 494/907 (54%) | 433/509 (85%) | 0/313 (0%) | 61/85 (72%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 543 atoms were assigned a chemical shift out of a possible 1193. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone | 220/452 (49%) | 151/184 (82%) | 0/182 (0%) | 69/86 (80%) |
| Sidechain | 316/676 (47%) | 315/446 (71%) | 0/206 (0%) | 1/24 (4%) |
| Aromatic | 7/65 (11%) | 7/33 (21%) | 0/29 (0%) | 0/3 (0%) |
| Overall | 543/1193 (46%) | 473/663 (71%) | 0/417 (0%) | 70/113 (62%) |

7.4.4 Statistically unusual chemical shifts [i](#)

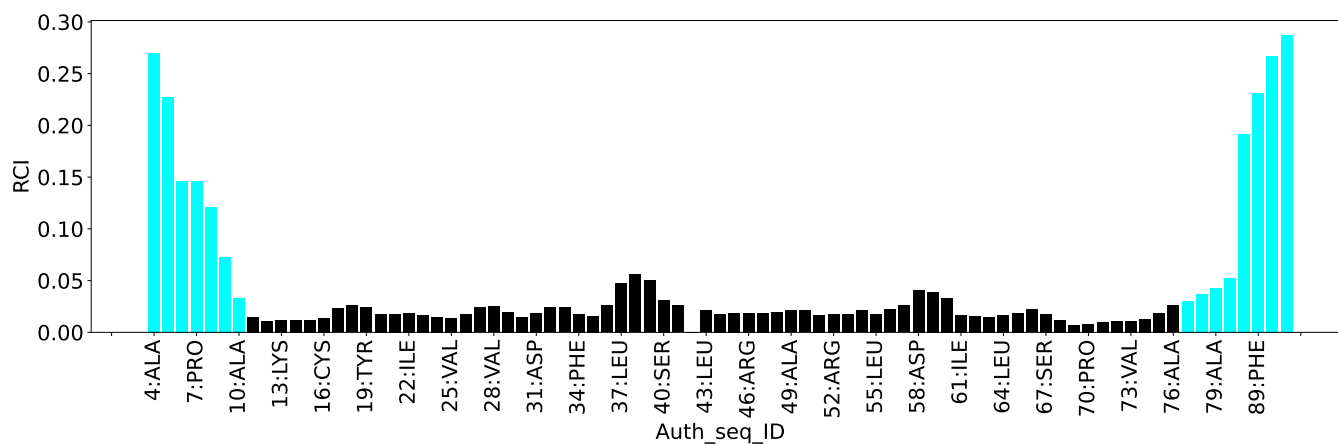
There are no statistically unusual chemical shifts.

7.4.5 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 | 1052 |
| Intra-residue ($ i-j =0$) | 322 |
| Sequential ($ i-j =1$) | 265 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 244 |
| Long range ($ i-j \geq 5$) | 221 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 150 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 13.2 |
| Number of long range restraints per residue ¹ | 2.4 |

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small) | 16.5 | 0.2 |
| 0.2-0.5 (Medium) | 27.1 | 0.5 |
| >0.5 (Large) | 27.6 | 2.85 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 7.0 | 9.83 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

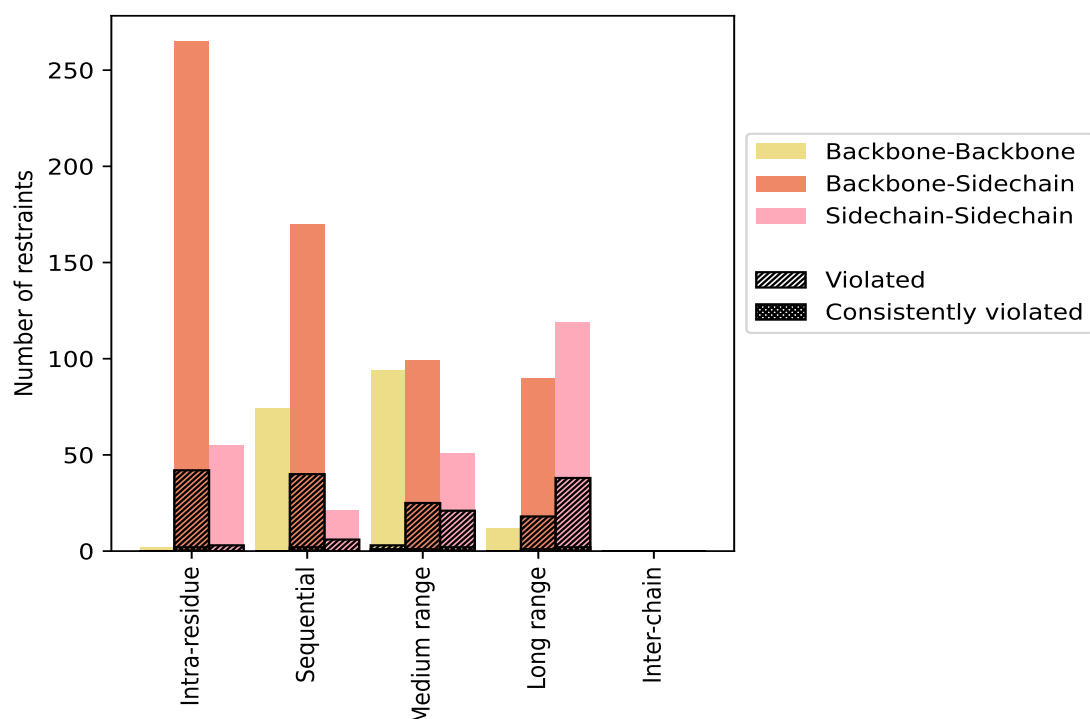
9.1 Summary of distance violations ⓘ

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 322 | 30.6 | 45 | 14.0 | 4.3 | 2 | 0.6 | 0.2 |
| Backbone-Backbone | 2 | 0.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 265 | 25.2 | 42 | 15.8 | 4.0 | 2 | 0.8 | 0.2 |
| Sidechain-Sidechain | 55 | 5.2 | 3 | 5.5 | 0.3 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 265 | 25.2 | 46 | 17.4 | 4.4 | 2 | 0.8 | 0.2 |
| Backbone-Backbone | 74 | 7.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 170 | 16.2 | 40 | 23.5 | 3.8 | 2 | 1.2 | 0.2 |
| Sidechain-Sidechain | 21 | 2.0 | 6 | 28.6 | 0.6 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 244 | 23.2 | 49 | 20.1 | 4.7 | 4 | 1.6 | 0.4 |
| Backbone-Backbone | 94 | 8.9 | 3 | 3.2 | 0.3 | 1 | 1.1 | 0.1 |
| Backbone-Sidechain | 99 | 9.4 | 25 | 25.3 | 2.4 | 1 | 1.0 | 0.1 |
| Sidechain-Sidechain | 51 | 4.8 | 21 | 41.2 | 2.0 | 2 | 3.9 | 0.2 |
| Long range ($i-j \geq 5$) | 221 | 21.0 | 56 | 25.3 | 5.3 | 3 | 1.4 | 0.3 |
| Backbone-Backbone | 12 | 1.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 90 | 8.6 | 18 | 20.0 | 1.7 | 1 | 1.1 | 0.1 |
| Sidechain-Sidechain | 119 | 11.3 | 38 | 31.9 | 3.6 | 2 | 1.7 | 0.2 |
| 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 | 1052 | 100.0 | 196 | 18.6 | 18.6 | 11 | 1.0 | 1.0 |
| Backbone-Backbone | 182 | 17.3 | 3 | 1.6 | 0.3 | 1 | 0.5 | 0.1 |
| Backbone-Sidechain | 624 | 59.3 | 125 | 20.0 | 11.9 | 6 | 1.0 | 0.6 |
| Sidechain-Sidechain | 246 | 23.4 | 68 | 27.6 | 6.5 | 4 | 1.6 | 0.4 |

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

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



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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 13 | 19 | 12 | 21 | 0 | 65 | 0.53 | 1.44 | 0.38 | 0.38 |
| 2 | 15 | 14 | 13 | 21 | 0 | 63 | 0.45 | 1.55 | 0.36 | 0.35 |
| 3 | 17 | 19 | 16 | 30 | 0 | 82 | 0.59 | 2.54 | 0.46 | 0.46 |
| 4 | 14 | 16 | 15 | 28 | 0 | 73 | 0.53 | 1.93 | 0.45 | 0.39 |
| 5 | 15 | 13 | 16 | 24 | 0 | 68 | 0.54 | 2.7 | 0.46 | 0.43 |
| 6 | 12 | 16 | 10 | 17 | 0 | 55 | 0.52 | 1.9 | 0.43 | 0.36 |
| 7 | 12 | 16 | 12 | 22 | 0 | 62 | 0.53 | 2.46 | 0.44 | 0.4 |
| 8 | 14 | 17 | 13 | 25 | 0 | 69 | 0.47 | 1.89 | 0.44 | 0.31 |
| 9 | 13 | 19 | 12 | 21 | 0 | 65 | 0.55 | 2.55 | 0.5 | 0.36 |
| 10 | 15 | 16 | 18 | 28 | 0 | 77 | 0.54 | 2.72 | 0.46 | 0.38 |

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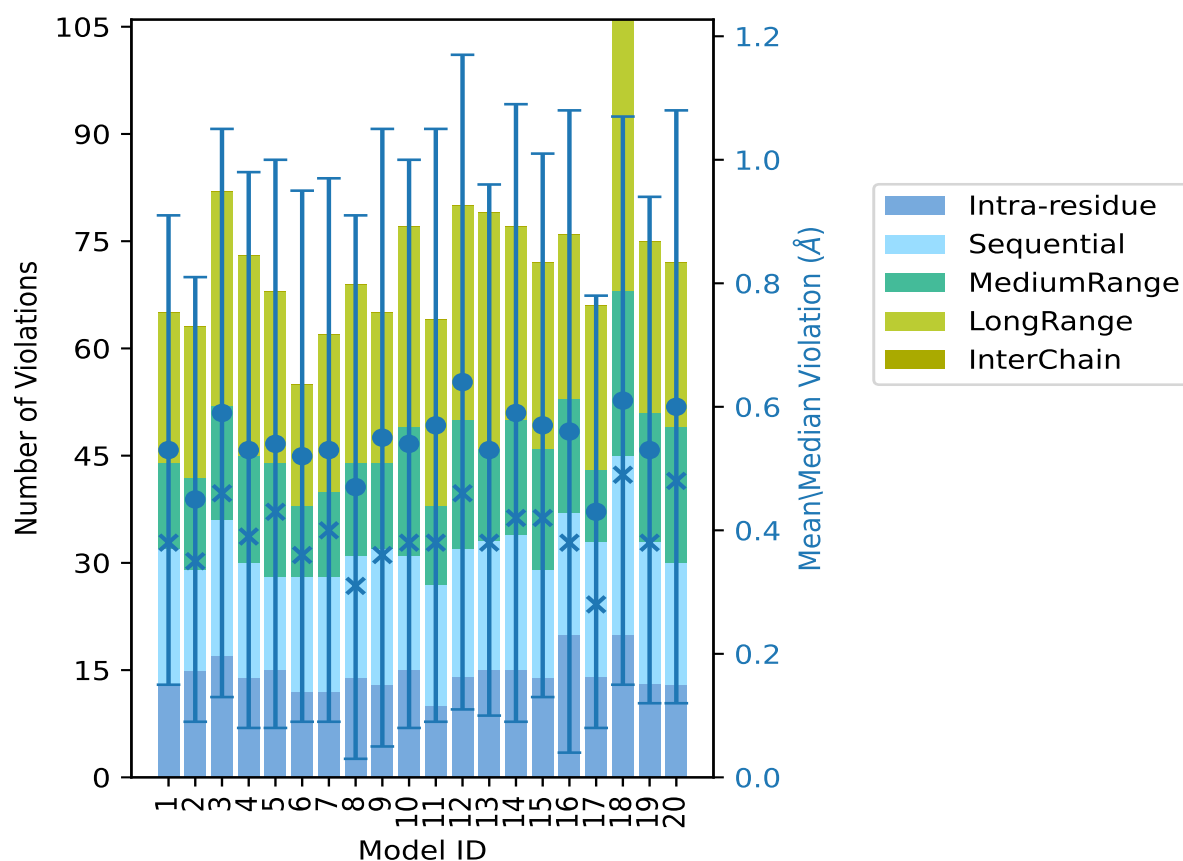
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 10 | 17 | 11 | 26 | 0 | 64 | 0.57 | 2.35 | 0.48 | 0.38 |
| 12 | 14 | 18 | 18 | 30 | 0 | 80 | 0.64 | 2.73 | 0.53 | 0.46 |
| 13 | 15 | 18 | 13 | 33 | 0 | 79 | 0.53 | 2.04 | 0.43 | 0.38 |
| 14 | 15 | 19 | 16 | 27 | 0 | 77 | 0.59 | 2.37 | 0.5 | 0.42 |
| 15 | 14 | 15 | 17 | 26 | 0 | 72 | 0.57 | 2.27 | 0.44 | 0.42 |
| 16 | 20 | 17 | 16 | 23 | 0 | 76 | 0.56 | 2.85 | 0.52 | 0.38 |
| 17 | 14 | 19 | 10 | 23 | 0 | 66 | 0.43 | 1.5 | 0.35 | 0.28 |
| 18 | 20 | 25 | 23 | 38 | 0 | 106 | 0.61 | 1.86 | 0.46 | 0.49 |
| 19 | 13 | 20 | 18 | 24 | 0 | 75 | 0.53 | 1.63 | 0.41 | 0.38 |
| 20 | 13 | 17 | 19 | 23 | 0 | 72 | 0.6 | 2.83 | 0.48 | 0.48 |

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

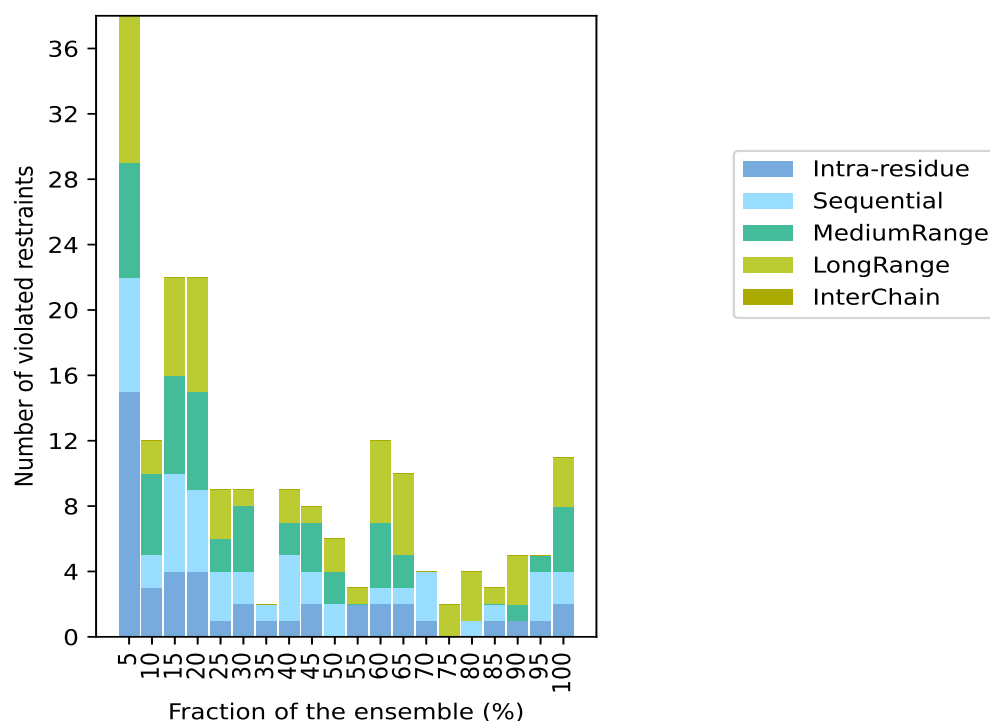
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 856(IR:277, SQ:219, MR:195, LR:165, IC:0) restraints are 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 | % |
| 15 | 7 | 7 | 9 | 0 | 38 | 1 | 5.0 |
| 3 | 2 | 5 | 2 | 0 | 12 | 2 | 10.0 |
| 4 | 6 | 6 | 6 | 0 | 22 | 3 | 15.0 |
| 4 | 5 | 6 | 7 | 0 | 22 | 4 | 20.0 |
| 1 | 3 | 2 | 3 | 0 | 9 | 5 | 25.0 |
| 2 | 2 | 4 | 1 | 0 | 9 | 6 | 30.0 |
| 1 | 1 | 0 | 0 | 0 | 2 | 7 | 35.0 |
| 1 | 4 | 2 | 2 | 0 | 9 | 8 | 40.0 |
| 2 | 2 | 3 | 1 | 0 | 8 | 9 | 45.0 |
| 0 | 2 | 2 | 2 | 0 | 6 | 10 | 50.0 |
| 2 | 0 | 0 | 1 | 0 | 3 | 11 | 55.0 |
| 2 | 1 | 4 | 5 | 0 | 12 | 12 | 60.0 |
| 2 | 1 | 2 | 5 | 0 | 10 | 13 | 65.0 |
| 1 | 3 | 0 | 0 | 0 | 4 | 14 | 70.0 |
| 0 | 0 | 0 | 2 | 0 | 2 | 15 | 75.0 |
| 0 | 1 | 0 | 3 | 0 | 4 | 16 | 80.0 |
| 1 | 1 | 0 | 1 | 0 | 3 | 17 | 85.0 |
| 1 | 0 | 1 | 3 | 0 | 5 | 18 | 90.0 |
| 1 | 3 | 1 | 0 | 0 | 5 | 19 | 95.0 |
| 2 | 2 | 4 | 3 | 0 | 11 | 20 | 100.0 |

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

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

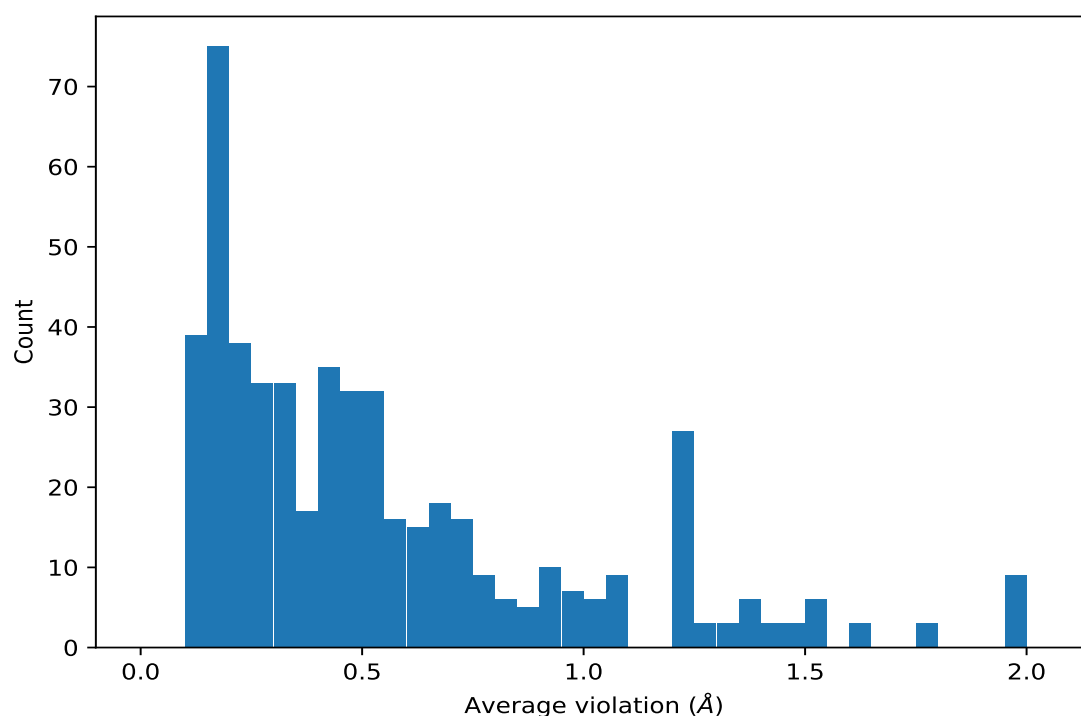
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 20 | 1.99 | 0.6 | 1.66 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 20 | 1.99 | 0.6 | 1.66 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 20 | 1.5 | 0.15 | 1.5 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 20 | 1.5 | 0.15 | 1.5 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 20 | 1.5 | 0.15 | 1.5 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 20 | 1.31 | 0.3 | 1.47 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 20 | 1.31 | 0.3 | 1.47 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 20 | 1.31 | 0.3 | 1.47 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 20 | 0.99 | 0.12 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 20 | 0.99 | 0.12 | 1.0 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 20 | 0.99 | 0.12 | 1.0 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 20 | 0.99 | 0.12 | 1.0 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 20 | 0.99 | 0.12 | 1.0 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 20 | 0.99 | 0.12 | 1.0 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 20 | 0.87 | 0.11 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 20 | 0.87 | 0.11 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 20 | 0.87 | 0.11 | 0.89 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 20 | 0.54 | 0.03 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 20 | 0.54 | 0.03 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 20 | 0.54 | 0.03 | 0.53 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 20 | 0.54 | 0.21 | 0.6 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 20 | 0.54 | 0.21 | 0.6 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 20 | 0.54 | 0.21 | 0.6 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 20 | 0.44 | 0.2 | 0.43 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 20 | 0.44 | 0.2 | 0.43 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 20 | 0.44 | 0.2 | 0.43 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 20 | 0.44 | 0.24 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 20 | 0.44 | 0.24 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 20 | 0.44 | 0.24 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD21 | 20 | 0.44 | 0.24 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD22 | 20 | 0.44 | 0.24 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD23 | 20 | 0.44 | 0.24 | 0.34 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 20 | 0.39 | 0.08 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 20 | 0.31 | 0.15 | 0.3 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 20 | 0.31 | 0.15 | 0.3 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 20 | 0.31 | 0.15 | 0.3 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 19 | 1.23 | 0.13 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 19 | 1.23 | 0.13 | 1.25 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 19 | 0.85 | 0.44 | 0.96 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 19 | 0.45 | 0.04 | 0.45 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 19 | 0.45 | 0.04 | 0.45 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 19 | 0.45 | 0.04 | 0.45 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 19 | 0.39 | 0.04 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 19 | 0.39 | 0.04 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 19 | 0.39 | 0.04 | 0.39 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 19 | 0.25 | 0.06 | 0.24 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 18 | 0.78 | 0.27 | 0.88 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 18 | 0.78 | 0.27 | 0.88 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 18 | 0.66 | 0.79 | 0.28 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 18 | 0.66 | 0.79 | 0.28 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 18 | 0.66 | 0.79 | 0.28 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 18 | 0.49 | 0.25 | 0.46 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 18 | 0.49 | 0.25 | 0.46 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 18 | 0.49 | 0.25 | 0.46 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD21 | 18 | 0.49 | 0.25 | 0.46 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD22 | 18 | 0.49 | 0.25 | 0.46 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD23 | 18 | 0.49 | 0.25 | 0.46 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 18 | 0.48 | 0.05 | 0.48 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 18 | 0.48 | 0.05 | 0.48 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 18 | 0.48 | 0.05 | 0.48 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 18 | 0.28 | 0.04 | 0.29 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 17 | 0.33 | 0.14 | 0.38 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 17 | 0.33 | 0.14 | 0.38 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 17 | 0.27 | 0.08 | 0.29 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 17 | 0.27 | 0.08 | 0.29 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 17 | 0.27 | 0.08 | 0.29 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 17 | 0.25 | 0.1 | 0.23 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 17 | 0.25 | 0.1 | 0.23 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 17 | 0.25 | 0.1 | 0.23 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 16 | 1.21 | 0.54 | 1.29 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 16 | 1.21 | 0.54 | 1.29 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 16 | 1.21 | 0.54 | 1.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 16 | 0.72 | 0.45 | 0.9 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 16 | 0.72 | 0.45 | 0.9 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 16 | 0.46 | 0.25 | 0.43 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 16 | 0.46 | 0.25 | 0.43 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 16 | 0.19 | 0.07 | 0.18 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 16 | 0.19 | 0.07 | 0.18 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 16 | 0.19 | 0.07 | 0.18 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 15 | 0.34 | 0.12 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 15 | 0.34 | 0.12 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 15 | 0.34 | 0.12 | 0.33 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 15 | 0.24 | 0.11 | 0.19 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 15 | 0.24 | 0.11 | 0.19 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 15 | 0.24 | 0.11 | 0.19 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 14 | 0.7 | 0.15 | 0.69 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 14 | 0.53 | 0.1 | 0.52 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 14 | 0.5 | 0.27 | 0.56 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 14 | 0.28 | 0.07 | 0.28 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 13 | 1.36 | 0.53 | 1.53 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 13 | 1.36 | 0.53 | 1.53 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 13 | 1.36 | 0.53 | 1.53 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 13 | 1.24 | 0.32 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 13 | 1.24 | 0.32 | 1.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 13 | 1.24 | 0.32 | 1.26 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 13 | 0.8 | 0.16 | 0.81 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 13 | 0.8 | 0.16 | 0.81 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 13 | 0.8 | 0.16 | 0.81 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 13 | 0.71 | 0.27 | 0.74 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 13 | 0.71 | 0.27 | 0.74 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 13 | 0.71 | 0.27 | 0.74 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 13 | 0.62 | 0.16 | 0.63 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 13 | 0.62 | 0.16 | 0.63 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 13 | 0.55 | 0.37 | 0.42 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 13 | 0.53 | 0.09 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 13 | 0.53 | 0.09 | 0.54 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 13 | 0.38 | 0.04 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 13 | 0.38 | 0.04 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 13 | 0.38 | 0.04 | 0.39 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 13 | 0.27 | 0.08 | 0.28 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 13 | 0.27 | 0.08 | 0.28 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 13 | 0.27 | 0.08 | 0.28 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 13 | 0.2 | 0.04 | 0.2 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 12 | 1.45 | 0.21 | 1.48 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 12 | 1.45 | 0.21 | 1.48 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 12 | 1.45 | 0.21 | 1.48 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 12 | 1.39 | 0.09 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 12 | 1.39 | 0.09 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 12 | 1.39 | 0.09 | 1.42 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 12 | 1.21 | 0.26 | 1.14 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 12 | 1.21 | 0.26 | 1.14 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 12 | 1.21 | 0.26 | 1.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 12 | 1.21 | 0.26 | 1.14 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 12 | 1.21 | 0.26 | 1.14 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 12 | 1.21 | 0.26 | 1.14 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 12 | 1.08 | 0.2 | 1.15 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 12 | 1.08 | 0.2 | 1.15 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 12 | 0.92 | 0.43 | 0.82 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 12 | 0.92 | 0.43 | 0.82 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 12 | 0.51 | 0.19 | 0.44 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 12 | 0.51 | 0.19 | 0.44 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 12 | 0.51 | 0.19 | 0.44 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 12 | 0.51 | 0.19 | 0.44 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 12 | 0.51 | 0.19 | 0.44 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 12 | 0.51 | 0.19 | 0.44 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 12 | 0.43 | 0.11 | 0.46 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 12 | 0.43 | 0.11 | 0.46 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 12 | 0.43 | 0.11 | 0.46 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 12 | 0.41 | 0.14 | 0.4 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 12 | 0.41 | 0.14 | 0.4 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 12 | 0.41 | 0.14 | 0.4 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 12 | 0.33 | 0.17 | 0.29 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 12 | 0.33 | 0.17 | 0.29 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 12 | 0.33 | 0.17 | 0.29 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 12 | 0.32 | 0.05 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 12 | 0.32 | 0.05 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 12 | 0.32 | 0.05 | 0.33 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 12 | 0.22 | 0.05 | 0.21 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 12 | 0.16 | 0.07 | 0.13 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 11 | 0.53 | 0.04 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 11 | 0.53 | 0.04 | 0.52 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 11 | 0.53 | 0.04 | 0.52 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 11 | 0.49 | 0.19 | 0.5 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 11 | 0.49 | 0.19 | 0.5 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 11 | 0.49 | 0.19 | 0.5 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 11 | 0.3 | 0.08 | 0.32 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 11 | 0.3 | 0.08 | 0.32 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 11 | 0.3 | 0.08 | 0.32 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 10 | 0.48 | 0.21 | 0.47 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 10 | 0.48 | 0.21 | 0.47 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 10 | 0.48 | 0.21 | 0.47 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 10 | 0.48 | 0.21 | 0.47 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 10 | 0.48 | 0.21 | 0.47 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 10 | 0.48 | 0.21 | 0.47 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 10 | 0.47 | 0.06 | 0.5 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 10 | 0.43 | 0.14 | 0.42 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 10 | 0.43 | 0.14 | 0.42 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 10 | 0.43 | 0.14 | 0.42 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 10 | 0.2 | 0.11 | 0.15 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 10 | 0.2 | 0.11 | 0.15 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 10 | 0.2 | 0.11 | 0.15 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 10 | 0.17 | 0.05 | 0.16 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 10 | 0.17 | 0.05 | 0.16 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 10 | 0.17 | 0.05 | 0.16 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 10 | 0.15 | 0.04 | 0.14 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 9 | 1.52 | 0.2 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 9 | 1.52 | 0.2 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 9 | 1.52 | 0.2 | 1.51 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 9 | 0.87 | 0.35 | 0.95 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 9 | 0.59 | 0.04 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 9 | 0.59 | 0.04 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 9 | 0.59 | 0.04 | 0.61 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 9 | 0.44 | 0.2 | 0.36 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 9 | 0.42 | 0.05 | 0.42 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 9 | 0.42 | 0.05 | 0.42 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 9 | 0.42 | 0.05 | 0.42 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 9 | 0.38 | 0.08 | 0.38 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 9 | 0.29 | 0.1 | 0.27 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 9 | 0.29 | 0.1 | 0.27 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 9 | 0.29 | 0.1 | 0.27 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 9 | 0.17 | 0.04 | 0.16 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 8 | 0.46 | 0.2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 8 | 0.44 | 0.12 | 0.48 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 8 | 0.25 | 0.08 | 0.26 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 8 | 0.25 | 0.08 | 0.26 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 8 | 0.25 | 0.08 | 0.26 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 8 | 0.25 | 0.08 | 0.26 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 8 | 0.25 | 0.08 | 0.26 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 8 | 0.25 | 0.08 | 0.26 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 8 | 0.21 | 0.04 | 0.2 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 8 | 0.2 | 0.09 | 0.18 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 8 | 0.2 | 0.09 | 0.18 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 8 | 0.19 | 0.06 | 0.19 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 8 | 0.19 | 0.06 | 0.19 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 8 | 0.19 | 0.06 | 0.19 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 8 | 0.18 | 0.06 | 0.16 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 8 | 0.17 | 0.03 | 0.16 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 8 | 0.14 | 0.02 | 0.14 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 8 | 0.14 | 0.02 | 0.14 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 8 | 0.14 | 0.02 | 0.14 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 7 | 0.32 | 0.12 | 0.27 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 7 | 0.26 | 0.17 | 0.18 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 7 | 0.26 | 0.17 | 0.18 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 6 | 0.69 | 0.28 | 0.74 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 6 | 0.69 | 0.28 | 0.74 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 6 | 0.69 | 0.28 | 0.74 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 6 | 0.51 | 0.2 | 0.56 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 6 | 0.36 | 0.25 | 0.34 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 6 | 0.36 | 0.25 | 0.34 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 6 | 0.36 | 0.25 | 0.34 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 6 | 0.36 | 0.25 | 0.34 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 6 | 0.36 | 0.25 | 0.34 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 6 | 0.36 | 0.25 | 0.34 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 6 | 0.26 | 0.28 | 0.14 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 6 | 0.26 | 0.28 | 0.14 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 6 | 0.26 | 0.28 | 0.14 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 6 | 0.21 | 0.07 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 6 | 0.19 | 0.08 | 0.17 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 6 | 0.19 | 0.08 | 0.17 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 6 | 0.19 | 0.08 | 0.17 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 6 | 0.19 | 0.05 | 0.18 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 6 | 0.19 | 0.05 | 0.18 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 6 | 0.16 | 0.04 | 0.18 |
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 6 | 0.14 | 0.02 | 0.14 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG11 | 5 | 0.69 | 0.47 | 0.54 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG12 | 5 | 0.69 | 0.47 | 0.54 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG13 | 5 | 0.69 | 0.47 | 0.54 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD21 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD22 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD23 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD21 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD22 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD23 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD21 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD22 | 5 | 0.68 | 0.08 | 0.69 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD23 | 5 | 0.68 | 0.08 | 0.69 |
| (1,195) | 1:13:A:LYS:HG3 | 1:14:A:VAL:H | 5 | 0.42 | 0.07 | 0.43 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG21 | 5 | 0.4 | 0.1 | 0.42 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG22 | 5 | 0.4 | 0.1 | 0.42 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG23 | 5 | 0.4 | 0.1 | 0.42 |
| (1,246) | 1:21:A:GLU:HG2 | 1:22:A:ILE:H | 5 | 0.3 | 0.08 | 0.28 |
| (1,924) | 1:62:A:ARG:HB3 | 1:63:A:GLN:HE21 | 5 | 0.22 | 0.08 | 0.2 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD21 | 5 | 0.2 | 0.08 | 0.17 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD22 | 5 | 0.2 | 0.08 | 0.17 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD23 | 5 | 0.2 | 0.08 | 0.17 |
| (1,373) | 1:53:A:GLU:H | 1:53:A:GLU:HG3 | 5 | 0.15 | 0.06 | 0.14 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG11 | 5 | 0.14 | 0.03 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG12 | 5 | 0.14 | 0.03 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG13 | 5 | 0.14 | 0.03 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 5 | 0.14 | 0.03 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 5 | 0.14 | 0.03 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 5 | 0.14 | 0.03 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG21 | 4 | 1.76 | 0.12 | 1.79 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG22 | 4 | 1.76 | 0.12 | 1.79 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG23 | 4 | 1.76 | 0.12 | 1.79 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG21 | 4 | 1.64 | 0.04 | 1.62 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG22 | 4 | 1.64 | 0.04 | 1.62 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG23 | 4 | 1.64 | 0.04 | 1.62 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG21 | 4 | 1.41 | 0.17 | 1.36 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG22 | 4 | 1.41 | 0.17 | 1.36 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG23 | 4 | 1.41 | 0.17 | 1.36 |
| (1,1011) | 1:28:A:VAL:HG11 | 1:32:A:ASP:H | 4 | 1.28 | 0.21 | 1.24 |
| (1,1011) | 1:28:A:VAL:HG12 | 1:32:A:ASP:H | 4 | 1.28 | 0.21 | 1.24 |
| (1,1011) | 1:28:A:VAL:HG13 | 1:32:A:ASP:H | 4 | 1.28 | 0.21 | 1.24 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG11 | 4 | 1.0 | 0.04 | 1.0 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG12 | 4 | 1.0 | 0.04 | 1.0 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG13 | 4 | 1.0 | 0.04 | 1.0 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG11 | 4 | 1.0 | 0.04 | 1.0 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG12 | 4 | 1.0 | 0.04 | 1.0 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG13 | 4 | 1.0 | 0.04 | 1.0 |
| (1,867) | 1:7:A:PRO:HA | 1:8:A:GLU:HB2 | 4 | 0.99 | 0.08 | 1.01 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG21 | 4 | 0.83 | 0.11 | 0.88 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG22 | 4 | 0.83 | 0.11 | 0.88 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG23 | 4 | 0.83 | 0.11 | 0.88 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG21 | 4 | 0.63 | 0.39 | 0.61 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG22 | 4 | 0.63 | 0.39 | 0.61 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG23 | 4 | 0.63 | 0.39 | 0.61 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG11 | 4 | 0.57 | 0.04 | 0.57 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG12 | 4 | 0.57 | 0.04 | 0.57 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG13 | 4 | 0.57 | 0.04 | 0.57 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG11 | 4 | 0.57 | 0.04 | 0.57 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG12 | 4 | 0.57 | 0.04 | 0.57 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG13 | 4 | 0.57 | 0.04 | 0.57 |
| (1,853) | 1:91:A:LYS:HA | 1:91:A:LYS:HD3 | 4 | 0.52 | 0.42 | 0.38 |
| (1,743) | 1:28:A:VAL:HG11 | 1:70:A:PRO:HB3 | 4 | 0.51 | 0.2 | 0.5 |
| (1,743) | 1:28:A:VAL:HG12 | 1:70:A:PRO:HB3 | 4 | 0.51 | 0.2 | 0.5 |
| (1,743) | 1:28:A:VAL:HG13 | 1:70:A:PRO:HB3 | 4 | 0.51 | 0.2 | 0.5 |
| (1,110) | 1:62:A:ARG:HA | 1:62:A:ARG:HD2 | 4 | 0.4 | 0.06 | 0.4 |
| (1,110) | 1:62:A:ARG:HA | 1:62:A:ARG:HD3 | 4 | 0.4 | 0.06 | 0.4 |
| (1,576) | 1:12:A:GLU:H | 1:13:A:LYS:HG3 | 4 | 0.32 | 0.14 | 0.28 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG21 | 4 | 0.32 | 0.11 | 0.32 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG22 | 4 | 0.32 | 0.11 | 0.32 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG23 | 4 | 0.32 | 0.11 | 0.32 |
| (1,869) | 1:46:A:ARG:HA | 1:46:A:ARG:HD2 | 4 | 0.28 | 0.13 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD11 | 4 | 0.27 | 0.05 | 0.28 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD12 | 4 | 0.27 | 0.05 | 0.28 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD13 | 4 | 0.27 | 0.05 | 0.28 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD11 | 4 | 0.23 | 0.05 | 0.22 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD12 | 4 | 0.23 | 0.05 | 0.22 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD13 | 4 | 0.23 | 0.05 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 4 | 0.2 | 0.04 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 4 | 0.2 | 0.04 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 4 | 0.2 | 0.04 | 0.22 |
| (1,40) | 1:25:A:VAL:HG11 | 1:37:A:LEU:HB2 | 4 | 0.19 | 0.05 | 0.16 |
| (1,40) | 1:25:A:VAL:HG12 | 1:37:A:LEU:HB2 | 4 | 0.19 | 0.05 | 0.16 |
| (1,40) | 1:25:A:VAL:HG13 | 1:37:A:LEU:HB2 | 4 | 0.19 | 0.05 | 0.16 |
| (1,443) | 1:62:A:ARG:HB3 | 1:64:A:LEU:H | 4 | 0.18 | 0.04 | 0.18 |
| (1,699) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:23:A:LEU:HD21 | 1:37:A:LEU:H | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:23:A:LEU:HD22 | 1:37:A:LEU:H | 4 | 0.18 | 0.06 | 0.18 |
| (1,699) | 1:23:A:LEU:HD23 | 1:37:A:LEU:H | 4 | 0.18 | 0.06 | 0.18 |
| (1,370) | 1:50:A:ARG:HB2 | 1:51:A:ILE:H | 4 | 0.17 | 0.07 | 0.15 |
| (1,94) | 1:18:A:LEU:HA | 1:21:A:GLU:HB2 | 3 | 0.94 | 0.1 | 0.92 |
| (1,4) | 1:15:A:LEU:HD11 | 1:74:A:ALA:HA | 3 | 0.71 | 0.02 | 0.7 |
| (1,4) | 1:15:A:LEU:HD12 | 1:74:A:ALA:HA | 3 | 0.71 | 0.02 | 0.7 |
| (1,4) | 1:15:A:LEU:HD13 | 1:74:A:ALA:HA | 3 | 0.71 | 0.02 | 0.7 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD11 | 3 | 0.6 | 0.35 | 0.39 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD12 | 3 | 0.6 | 0.35 | 0.39 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD13 | 3 | 0.6 | 0.35 | 0.39 |
| (1,910) | 1:75:A:ARG:HG3 | 1:76:A:ALA:H | 3 | 0.53 | 0.03 | 0.55 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD11 | 3 | 0.43 | 0.34 | 0.25 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD12 | 3 | 0.43 | 0.34 | 0.25 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD13 | 3 | 0.43 | 0.34 | 0.25 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 3 | 0.29 | 0.17 | 0.2 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 3 | 0.29 | 0.17 | 0.2 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 3 | 0.29 | 0.17 | 0.2 |
| (1,362) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 3 | 0.19 | 0.04 | 0.19 |
| (1,316) | 1:23:A:LEU:HD11 | 1:39:A:GLY:H | 3 | 0.18 | 0.04 | 0.19 |
| (1,316) | 1:23:A:LEU:HD12 | 1:39:A:GLY:H | 3 | 0.18 | 0.04 | 0.19 |
| (1,316) | 1:23:A:LEU:HD13 | 1:39:A:GLY:H | 3 | 0.18 | 0.04 | 0.19 |
| (1,202) | 1:15:A:LEU:HB3 | 1:16:A:CYS:H | 3 | 0.18 | 0.05 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB1 | 3 | 0.17 | 0.03 | 0.17 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB2 | 3 | 0.17 | 0.03 | 0.17 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB3 | 3 | 0.17 | 0.03 | 0.17 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD11 | 3 | 0.16 | 0.04 | 0.16 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD12 | 3 | 0.16 | 0.04 | 0.16 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD13 | 3 | 0.16 | 0.04 | 0.16 |
| (1,267) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 3 | 0.16 | 0.06 | 0.12 |
| (1,267) | 1:20:A:ALA:HB1 | 1:28:A:VAL:H | 3 | 0.16 | 0.06 | 0.12 |
| (1,267) | 1:20:A:ALA:HB2 | 1:28:A:VAL:H | 3 | 0.16 | 0.06 | 0.12 |
| (1,267) | 1:20:A:ALA:HB3 | 1:28:A:VAL:H | 3 | 0.16 | 0.06 | 0.12 |
| (1,209) | 1:21:A:GLU:HB2 | 1:22:A:ILE:H | 3 | 0.15 | 0.01 | 0.15 |
| (1,209) | 1:21:A:GLU:HB3 | 1:22:A:ILE:H | 3 | 0.15 | 0.01 | 0.15 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD11 | 3 | 0.15 | 0.05 | 0.13 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD12 | 3 | 0.15 | 0.05 | 0.13 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD13 | 3 | 0.15 | 0.05 | 0.13 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD11 | 3 | 0.15 | 0.05 | 0.13 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD12 | 3 | 0.15 | 0.05 | 0.13 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD13 | 3 | 0.15 | 0.05 | 0.13 |
| (1,249) | 1:22:A:ILE:H | 1:22:A:ILE:HG13 | 3 | 0.14 | 0.02 | 0.14 |
| (1,350) | 1:47:A:LEU:HD11 | 1:48:A:ILE:H | 3 | 0.14 | 0.03 | 0.13 |
| (1,350) | 1:47:A:LEU:HD12 | 1:48:A:ILE:H | 3 | 0.14 | 0.03 | 0.13 |
| (1,350) | 1:47:A:LEU:HD13 | 1:48:A:ILE:H | 3 | 0.14 | 0.03 | 0.13 |
| (1,418) | 1:54:A:GLU:HG3 | 1:55:A:LEU:H | 3 | 0.14 | 0.02 | 0.13 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 3 | 0.13 | 0.02 | 0.14 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 3 | 0.13 | 0.02 | 0.14 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 3 | 0.13 | 0.02 | 0.14 |
| (1,811) | 1:63:A:GLN:HA | 1:77:A:LEU:HB3 | 3 | 0.13 | 0.03 | 0.12 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB1 | 3 | 0.12 | 0.01 | 0.12 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB2 | 3 | 0.12 | 0.01 | 0.12 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB3 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG21 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG22 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG23 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG21 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG22 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG23 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG21 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG22 | 3 | 0.12 | 0.01 | 0.12 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG23 | 3 | 0.12 | 0.01 | 0.12 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD1 | 3 | 0.11 | 0.0 | 0.11 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD1 | 3 | 0.11 | 0.0 | 0.11 |

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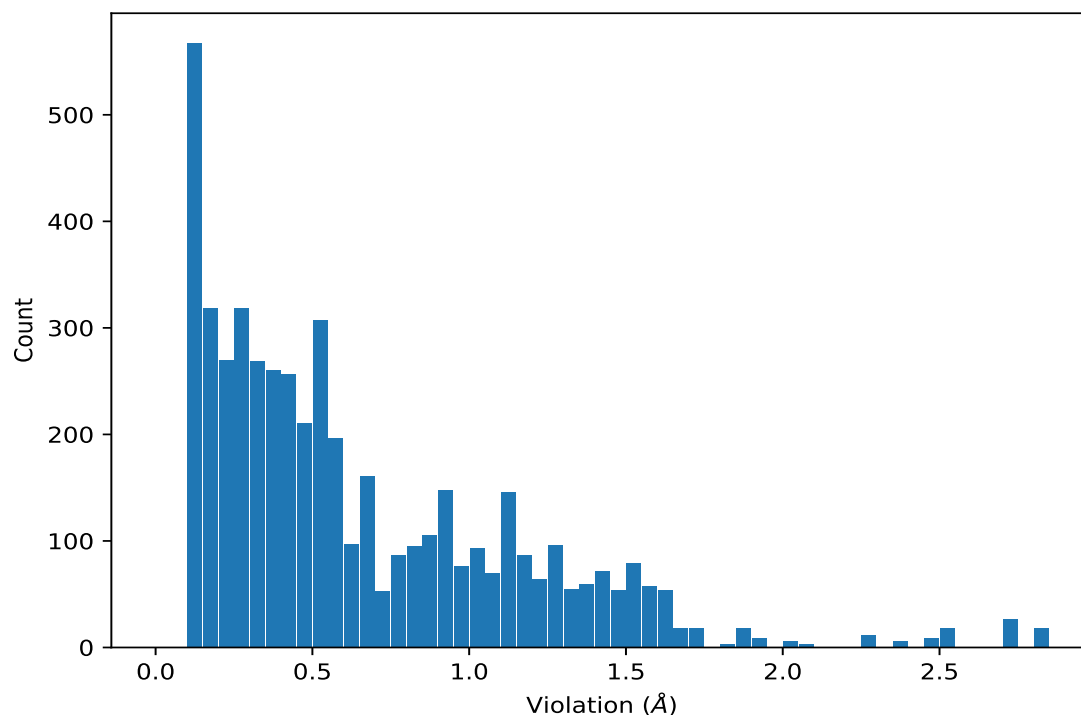
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD1 | 3 | 0.11 | 0.0 | 0.11 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,717) | 1:28:A:VAL:HG11 | 1:32:A:ASP:HB3 | 2 | 0.56 | 0.06 | 0.56 |
| (1,717) | 1:28:A:VAL:HG12 | 1:32:A:ASP:HB3 | 2 | 0.56 | 0.06 | 0.56 |
| (1,717) | 1:28:A:VAL:HG13 | 1:32:A:ASP:HB3 | 2 | 0.56 | 0.06 | 0.56 |
| (1,717) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 2 | 0.56 | 0.06 | 0.56 |
| (1,717) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 2 | 0.56 | 0.06 | 0.56 |
| (1,717) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 2 | 0.56 | 0.06 | 0.56 |
| (1,742) | 1:28:A:VAL:HG11 | 1:32:A:ASP:HB2 | 2 | 0.44 | 0.32 | 0.44 |
| (1,742) | 1:28:A:VAL:HG12 | 1:32:A:ASP:HB2 | 2 | 0.44 | 0.32 | 0.44 |
| (1,742) | 1:28:A:VAL:HG13 | 1:32:A:ASP:HB2 | 2 | 0.44 | 0.32 | 0.44 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG21 | 2 | 0.38 | 0.16 | 0.38 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG22 | 2 | 0.38 | 0.16 | 0.38 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG23 | 2 | 0.38 | 0.16 | 0.38 |
| (1,731) | 1:51:A:ILE:HG21 | 1:52:A:ARG:HG3 | 2 | 0.34 | 0.13 | 0.34 |
| (1,731) | 1:51:A:ILE:HG22 | 1:52:A:ARG:HG3 | 2 | 0.34 | 0.13 | 0.34 |
| (1,731) | 1:51:A:ILE:HG23 | 1:52:A:ARG:HG3 | 2 | 0.34 | 0.13 | 0.34 |
| (1,125) | 1:27:A:ARG:HB2 | 1:27:A:ARG:HD2 | 2 | 0.24 | 0.03 | 0.24 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD21 | 2 | 0.23 | 0.03 | 0.23 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD22 | 2 | 0.23 | 0.03 | 0.23 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD23 | 2 | 0.23 | 0.03 | 0.23 |
| (1,408) | 1:57:A:VAL:HG21 | 1:59:A:LEU:H | 2 | 0.21 | 0.01 | 0.21 |
| (1,408) | 1:57:A:VAL:HG22 | 1:59:A:LEU:H | 2 | 0.21 | 0.01 | 0.21 |
| (1,408) | 1:57:A:VAL:HG23 | 1:59:A:LEU:H | 2 | 0.21 | 0.01 | 0.21 |
| (1,269) | 1:26:A:GLU:HB2 | 1:27:A:ARG:H | 2 | 0.2 | 0.07 | 0.2 |
| (1,269) | 1:26:A:GLU:HB3 | 1:27:A:ARG:H | 2 | 0.2 | 0.07 | 0.2 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG21 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG22 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG23 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG21 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG22 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG23 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG21 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG22 | 2 | 0.15 | 0.02 | 0.15 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG23 | 2 | 0.15 | 0.02 | 0.15 |
| (1,1034) | 1:42:A:ALA:HA | 1:45:A:MET:HG2 | 2 | 0.15 | 0.04 | 0.15 |
| (1,519) | 1:27:A:ARG:H | 1:27:A:ARG:HB3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,784) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 16 | 2.85 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 20 | 2.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 20 | 2.83 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 12 | 2.73 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 10 | 2.72 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 5 | 2.7 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 9 | 2.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 9 | 2.55 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 3 | 2.54 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 7 | 2.46 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 7 | 2.46 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 14 | 2.37 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 14 | 2.37 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 14 | 2.37 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 11 | 2.35 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 11 | 2.35 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 11 | 2.35 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 12 | 2.28 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 12 | 2.28 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 12 | 2.28 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 15 | 2.27 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 15 | 2.27 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 14 | 2.09 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 14 | 2.09 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 14 | 2.09 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 13 | 2.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 13 | 2.04 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 13 | 2.04 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 20 | 2.03 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 20 | 2.03 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 20 | 2.03 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 4 | 1.93 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 4 | 1.93 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 6 | 1.9 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 6 | 1.9 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 6 | 1.9 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 8 | 1.89 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 8 | 1.89 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 8 | 1.89 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG21 | 5 | 1.88 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG22 | 5 | 1.88 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG23 | 5 | 1.88 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 16 | 1.86 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 16 | 1.86 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 16 | 1.86 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 18 | 1.86 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 18 | 1.86 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 18 | 1.86 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG21 | 12 | 1.86 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG22 | 12 | 1.86 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG23 | 12 | 1.86 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 16 | 1.81 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 16 | 1.81 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 16 | 1.81 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 9 | 1.74 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 9 | 1.74 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 9 | 1.74 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 20 | 1.72 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 20 | 1.72 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 20 | 1.72 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG21 | 11 | 1.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG22 | 11 | 1.72 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG23 | 11 | 1.72 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 14 | 1.71 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 14 | 1.71 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG21 | 18 | 1.7 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG22 | 18 | 1.7 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG23 | 18 | 1.7 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 16 | 1.7 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 16 | 1.7 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 16 | 1.7 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 10 | 1.69 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 10 | 1.69 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 10 | 1.69 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 3 | 1.69 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 3 | 1.69 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 3 | 1.69 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 12 | 1.69 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 12 | 1.69 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 12 | 1.69 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG21 | 18 | 1.68 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG22 | 18 | 1.68 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG23 | 18 | 1.68 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 14 | 1.65 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 14 | 1.65 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 14 | 1.65 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 18 | 1.65 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 18 | 1.65 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 18 | 1.65 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG21 | 13 | 1.64 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG22 | 13 | 1.64 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG23 | 13 | 1.64 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 4 | 1.64 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 4 | 1.64 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 4 | 1.64 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 20 | 1.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 20 | 1.64 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 20 | 1.64 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 19 | 1.63 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 19 | 1.63 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 19 | 1.63 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 6 | 1.62 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 6 | 1.62 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 6 | 1.62 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 9 | 1.62 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 9 | 1.62 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 9 | 1.62 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 16 | 1.62 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 16 | 1.62 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 16 | 1.62 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 16 | 1.62 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 16 | 1.62 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 16 | 1.62 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 19 | 1.62 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 19 | 1.62 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG21 | 11 | 1.61 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG22 | 11 | 1.61 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG23 | 11 | 1.61 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 18 | 1.61 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 18 | 1.61 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 18 | 1.61 |
| (1,1011) | 1:28:A:VAL:HG11 | 1:32:A:ASP:H | 18 | 1.6 |
| (1,1011) | 1:28:A:VAL:HG12 | 1:32:A:ASP:H | 18 | 1.6 |
| (1,1011) | 1:28:A:VAL:HG13 | 1:32:A:ASP:H | 18 | 1.6 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 9 | 1.6 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 9 | 1.6 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 9 | 1.6 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 8 | 1.6 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 8 | 1.6 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 8 | 1.6 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 14 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 14 | 1.59 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 14 | 1.59 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG21 | 12 | 1.59 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG22 | 12 | 1.59 |
| (1,1004) | 1:27:A:ARG:HA | 1:28:A:VAL:HG23 | 12 | 1.59 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 18 | 1.59 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 18 | 1.59 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 18 | 1.59 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 4 | 1.59 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 4 | 1.59 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 4 | 1.59 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 18 | 1.58 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 18 | 1.58 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 18 | 1.58 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 18 | 1.58 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 18 | 1.58 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 18 | 1.58 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG21 | 15 | 1.58 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG22 | 15 | 1.58 |
| (1,399) | 1:55:A:LEU:H | 1:57:A:VAL:HG23 | 15 | 1.58 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 14 | 1.57 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 14 | 1.57 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 14 | 1.57 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 12 | 1.57 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 12 | 1.57 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 12 | 1.57 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 12 | 1.57 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 12 | 1.57 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 7 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 3 | 1.56 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 3 | 1.56 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 3 | 1.56 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 13 | 1.56 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 13 | 1.56 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 13 | 1.56 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 2 | 1.55 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 2 | 1.55 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 3 | 1.54 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 3 | 1.54 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 15 | 1.54 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 15 | 1.54 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 16 | 1.54 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 16 | 1.54 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 16 | 1.54 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 6 | 1.54 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 6 | 1.54 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 6 | 1.54 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 4 | 1.54 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 15 | 1.54 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 15 | 1.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 15 | 1.54 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 11 | 1.54 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 11 | 1.54 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 3 | 1.53 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 3 | 1.53 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 3 | 1.53 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 19 | 1.53 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 19 | 1.53 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 19 | 1.53 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 12 | 1.52 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 12 | 1.52 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 12 | 1.52 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 14 | 1.52 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 14 | 1.52 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 14 | 1.52 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 14 | 1.52 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 14 | 1.52 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 14 | 1.52 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 10 | 1.51 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 10 | 1.51 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 10 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 5 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 5 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 5 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 16 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 16 | 1.51 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 16 | 1.51 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 20 | 1.5 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 20 | 1.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 20 | 1.5 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 17 | 1.5 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 17 | 1.5 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 7 | 1.49 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 7 | 1.49 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 7 | 1.49 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 19 | 1.49 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 19 | 1.49 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 19 | 1.49 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 16 | 1.49 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 16 | 1.49 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 16 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 3 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 3 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 3 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 4 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 4 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 4 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 16 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 16 | 1.49 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 16 | 1.49 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 6 | 1.49 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 6 | 1.49 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 10 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 10 | 1.48 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 10 | 1.48 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 14 | 1.48 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 14 | 1.48 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 14 | 1.48 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 18 | 1.48 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 18 | 1.48 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 18 | 1.48 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 2 | 1.48 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 2 | 1.48 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 2 | 1.48 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 9 | 1.47 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 9 | 1.47 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 9 | 1.47 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 8 | 1.46 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 8 | 1.46 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 8 | 1.46 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 10 | 1.46 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 10 | 1.46 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 10 | 1.46 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 4 | 1.45 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 18 | 1.45 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 18 | 1.45 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 11 | 1.44 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 11 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 11 | 1.44 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 17 | 1.44 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 17 | 1.44 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 17 | 1.44 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 3 | 1.44 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 3 | 1.44 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 3 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 1 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 1 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 1 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 14 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 14 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 14 | 1.44 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 19 | 1.43 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 19 | 1.43 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 19 | 1.43 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 8 | 1.43 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 8 | 1.43 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 3 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 3 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 3 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 18 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 18 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 8 | 1.42 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 18 | 1.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 18 | 1.42 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 18 | 1.42 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 13 | 1.41 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 13 | 1.41 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 13 | 1.41 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 7 | 1.4 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 7 | 1.4 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 7 | 1.4 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 6 | 1.4 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 6 | 1.4 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 2 | 1.39 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 2 | 1.39 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 2 | 1.39 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 6 | 1.39 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 6 | 1.39 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 6 | 1.39 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 9 | 1.39 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 9 | 1.39 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 9 | 1.39 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG21 | 12 | 1.39 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG22 | 12 | 1.39 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG23 | 12 | 1.39 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 15 | 1.38 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 15 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 15 | 1.38 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 10 | 1.38 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 10 | 1.38 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 10 | 1.38 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 9 | 1.38 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 9 | 1.38 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 9 | 1.38 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 9 | 1.38 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 9 | 1.38 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 9 | 1.38 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 13 | 1.38 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 13 | 1.38 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 8 | 1.37 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 8 | 1.37 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 8 | 1.37 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 7 | 1.37 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 7 | 1.37 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 7 | 1.37 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 3 | 1.36 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 3 | 1.36 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 3 | 1.36 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 18 | 1.34 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 18 | 1.34 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 7 | 1.34 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 7 | 1.34 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 7 | 1.34 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 1 | 1.33 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 1 | 1.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 1 | 1.33 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG21 | 13 | 1.33 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG22 | 13 | 1.33 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG23 | 13 | 1.33 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 14 | 1.33 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 14 | 1.33 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD11 | 10 | 1.33 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD12 | 10 | 1.33 |
| (1,41) | 1:39:A:GLY:HA3 | 1:43:A:LEU:HD13 | 10 | 1.33 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 2 | 1.32 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 2 | 1.32 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 2 | 1.32 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 4 | 1.31 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 4 | 1.31 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 4 | 1.31 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 11 | 1.31 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 1 | 1.31 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 1 | 1.31 |
| (1,1011) | 1:28:A:VAL:HG11 | 1:32:A:ASP:H | 13 | 1.3 |
| (1,1011) | 1:28:A:VAL:HG12 | 1:32:A:ASP:H | 13 | 1.3 |
| (1,1011) | 1:28:A:VAL:HG13 | 1:32:A:ASP:H | 13 | 1.3 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 5 | 1.3 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 5 | 1.3 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 5 | 1.3 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 8 | 1.3 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 8 | 1.3 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 8 | 1.3 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 6 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 6 | 1.29 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 6 | 1.29 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 13 | 1.29 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 13 | 1.29 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 13 | 1.29 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 9 | 1.29 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 19 | 1.28 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 19 | 1.28 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 20 | 1.28 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG11 | 11 | 1.28 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG12 | 11 | 1.28 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG13 | 11 | 1.28 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 12 | 1.27 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 12 | 1.27 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 8 | 1.27 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 8 | 1.27 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 8 | 1.27 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 18 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 18 | 1.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 18 | 1.26 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD21 | 15 | 1.26 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD22 | 15 | 1.26 |
| (1,790) | 1:19:A:TYR:HB2 | 1:23:A:LEU:HD23 | 15 | 1.26 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 17 | 1.26 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 17 | 1.26 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 18 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 10 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 11 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 12 | 1.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 12 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 19 | 1.25 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 19 | 1.25 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 1 | 1.24 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 1 | 1.24 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 20 | 1.24 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 20 | 1.24 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 20 | 1.24 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 3 | 1.24 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 3 | 1.24 |
| (1,853) | 1:91:A:LYS:HA | 1:91:A:LYS:HD3 | 1 | 1.23 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 3 | 1.23 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 3 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 13 | 1.23 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 13 | 1.23 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 8 | 1.23 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 8 | 1.23 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 8 | 1.23 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 8 | 1.23 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 8 | 1.23 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 8 | 1.23 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG21 | 11 | 1.23 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG22 | 11 | 1.23 |
| (1,254) | 1:21:A:GLU:H | 1:28:A:VAL:HG23 | 11 | 1.23 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 4 | 1.21 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 4 | 1.21 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 4 | 1.21 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 4 | 1.21 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 4 | 1.21 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 4 | 1.21 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 20 | 1.21 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 20 | 1.21 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 20 | 1.21 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 20 | 1.21 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 20 | 1.21 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 20 | 1.21 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 1 | 1.21 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 1 | 1.21 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 1 | 1.21 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 4 | 1.2 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 4 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 17 | 1.2 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 17 | 1.2 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 17 | 1.2 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 12 | 1.2 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 12 | 1.2 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG11 | 14 | 1.2 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG12 | 14 | 1.2 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG13 | 14 | 1.2 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 4 | 1.19 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 16 | 1.19 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 16 | 1.19 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 17 | 1.19 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 17 | 1.19 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 17 | 1.19 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 13 | 1.18 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 13 | 1.18 |
| (1,1011) | 1:28:A:VAL:HG11 | 1:32:A:ASP:H | 12 | 1.18 |
| (1,1011) | 1:28:A:VAL:HG12 | 1:32:A:ASP:H | 12 | 1.18 |
| (1,1011) | 1:28:A:VAL:HG13 | 1:32:A:ASP:H | 12 | 1.18 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG21 | 15 | 1.18 |
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG22 | 15 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,503) | 1:72:A:GLY:H | 1:73:A:VAL:HG23 | 15 | 1.18 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 19 | 1.17 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 19 | 1.17 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 15 | 1.17 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 15 | 1.17 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 15 | 1.17 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 2 | 1.16 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 2 | 1.16 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 15 | 1.16 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 15 | 1.16 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 15 | 1.16 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 15 | 1.16 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 15 | 1.16 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 15 | 1.16 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 17 | 1.16 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 19 | 1.16 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 15 | 1.16 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 15 | 1.16 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 15 | 1.16 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG21 | 12 | 1.16 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG22 | 12 | 1.16 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG23 | 12 | 1.16 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 1 | 1.15 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 1 | 1.15 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 1 | 1.15 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 10 | 1.15 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 10 | 1.15 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 10 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 10 | 1.15 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 10 | 1.15 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 10 | 1.15 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 18 | 1.15 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 1 | 1.15 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 1 | 1.15 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 5 | 1.15 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 5 | 1.15 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 13 | 1.14 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 13 | 1.14 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 13 | 1.14 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 15 | 1.14 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 14 | 1.13 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 14 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 1 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 1 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 1 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 1 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 1 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 1 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 3 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 3 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 3 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 3 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 3 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 3 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 4 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 4 | 1.13 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 4 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 4 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 4 | 1.13 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD11 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD12 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD11 | 1:43:A:LEU:HD13 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD11 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD12 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD12 | 1:43:A:LEU:HD13 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD11 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD12 | 4 | 1.13 |
| (1,13) | 1:23:A:LEU:HD13 | 1:43:A:LEU:HD13 | 4 | 1.13 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 2 | 1.12 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 9 | 1.12 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 9 | 1.12 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 9 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 9 | 1.11 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 9 | 1.11 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 7 | 1.11 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 15 | 1.11 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 15 | 1.11 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 12 | 1.11 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 12 | 1.11 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD11 | 18 | 1.1 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD12 | 18 | 1.1 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD13 | 18 | 1.1 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 9 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 9 | 1.1 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 9 | 1.1 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD21 | 1 | 1.1 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD22 | 1 | 1.1 |
| (1,768) | 1:34:A:PHE:HB2 | 1:37:A:LEU:HD23 | 1 | 1.1 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 16 | 1.1 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 16 | 1.1 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 6 | 1.09 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 6 | 1.09 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 6 | 1.09 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 6 | 1.09 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 6 | 1.09 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 6 | 1.09 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 8 | 1.09 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 8 | 1.09 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 20 | 1.09 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 20 | 1.09 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 5 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 5 | 1.09 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 5 | 1.09 |
| (1,867) | 1:7:A:PRO:HA | 1:8:A:GLU:HB2 | 19 | 1.08 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 5 | 1.08 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 5 | 1.07 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 5 | 1.07 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 9 | 1.07 |
| (1,94) | 1:18:A:LEU:HA | 1:21:A:GLU:HB2 | 18 | 1.07 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 9 | 1.06 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 9 | 1.06 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 9 | 1.06 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 9 | 1.06 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 9 | 1.06 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 9 | 1.06 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 20 | 1.06 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 20 | 1.06 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 19 | 1.06 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 19 | 1.06 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 19 | 1.06 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 14 | 1.05 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 14 | 1.05 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 14 | 1.05 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 14 | 1.05 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 14 | 1.05 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 14 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,867) | 1:7:A:PRO:HA | 1:8:A:GLU:HB2 | 11 | 1.04 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG11 | 18 | 1.04 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG12 | 18 | 1.04 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG13 | 18 | 1.04 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG11 | 18 | 1.04 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG12 | 18 | 1.04 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG13 | 18 | 1.04 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD21 | 12 | 1.04 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD22 | 12 | 1.04 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD23 | 12 | 1.04 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 3 | 1.04 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 3 | 1.04 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 3 | 1.04 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD11 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD12 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB1 | 1:47:A:LEU:HD13 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD11 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD12 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB2 | 1:47:A:LEU:HD13 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD11 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD12 | 20 | 1.04 |
| (1,63) | 1:44:A:ALA:HB3 | 1:47:A:LEU:HD13 | 20 | 1.04 |
| (1,1011) | 1:28:A:VAL:HG11 | 1:32:A:ASP:H | 11 | 1.03 |
| (1,1011) | 1:28:A:VAL:HG12 | 1:32:A:ASP:H | 11 | 1.03 |
| (1,1011) | 1:28:A:VAL:HG13 | 1:32:A:ASP:H | 11 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 8 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 8 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 8 | 1.03 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 8 | 1.03 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 8 | 1.03 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 8 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 19 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 19 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 19 | 1.03 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 19 | 1.03 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 19 | 1.03 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 19 | 1.03 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG11 | 13 | 1.03 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG12 | 13 | 1.03 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG13 | 13 | 1.03 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG11 | 13 | 1.03 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG12 | 13 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG13 | 13 | 1.03 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 7 | 1.03 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 7 | 1.03 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 7 | 1.03 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 10 | 1.02 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 10 | 1.02 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 10 | 1.02 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 10 | 1.02 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 10 | 1.02 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 10 | 1.02 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 1 | 1.02 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 1 | 1.02 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 1 | 1.02 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 1 | 1.01 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 1 | 1.01 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 1 | 1.01 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 1 | 1.01 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 1 | 1.01 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 1 | 1.01 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 3 | 1.01 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 1 | 1.01 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 1 | 1.01 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 16 | 1.01 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 16 | 1.01 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 5 | 1.01 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 5 | 1.01 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 5 | 1.01 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 5 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 10 | 1.0 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 10 | 1.0 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 5 | 0.99 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 5 | 0.99 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 5 | 0.99 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 16 | 0.98 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 16 | 0.98 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 16 | 0.98 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 16 | 0.98 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 16 | 0.98 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 16 | 0.98 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 19 | 0.98 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 19 | 0.98 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 19 | 0.98 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 19 | 0.98 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 19 | 0.98 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 19 | 0.98 |
| (1,867) | 1:7:A:PRO:HA | 1:8:A:GLU:HB2 | 6 | 0.98 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 14 | 0.98 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 20 | 0.97 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 20 | 0.97 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 20 | 0.97 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 9 | 0.97 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 11 | 0.97 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 11 | 0.97 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 11 | 0.97 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD21 | 18 | 0.97 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD22 | 18 | 0.97 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD23 | 18 | 0.97 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 5 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 5 | 0.96 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 10 | 0.96 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 10 | 0.96 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG11 | 11 | 0.96 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG12 | 11 | 0.96 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG13 | 11 | 0.96 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG11 | 11 | 0.96 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG12 | 11 | 0.96 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG13 | 11 | 0.96 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG11 | 12 | 0.96 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG12 | 12 | 0.96 |
| (1,672) | 1:19:A:TYR:HE1 | 1:28:A:VAL:HG13 | 12 | 0.96 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG11 | 12 | 0.96 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG12 | 12 | 0.96 |
| (1,672) | 1:19:A:TYR:HE2 | 1:28:A:VAL:HG13 | 12 | 0.96 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 10 | 0.96 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 10 | 0.96 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 10 | 0.96 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 19 | 0.96 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 19 | 0.96 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 19 | 0.96 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 10 | 0.96 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 18 | 0.96 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 18 | 0.96 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 18 | 0.96 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 20 | 0.96 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 20 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 20 | 0.96 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 14 | 0.95 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 14 | 0.95 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 14 | 0.95 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 17 | 0.95 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 17 | 0.95 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 17 | 0.95 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 20 | 0.95 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 17 | 0.95 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 17 | 0.95 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 17 | 0.95 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 19 | 0.94 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 19 | 0.94 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 19 | 0.94 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 12 | 0.94 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 12 | 0.94 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 12 | 0.94 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 12 | 0.94 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 12 | 0.94 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 12 | 0.94 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 19 | 0.94 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 19 | 0.94 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 19 | 0.94 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 7 | 0.94 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 7 | 0.94 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 7 | 0.94 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 7 | 0.94 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 7 | 0.94 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 7 | 0.94 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 11 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 11 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 11 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 13 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 13 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 13 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 16 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 16 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 16 | 0.93 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 2 | 0.93 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 2 | 0.93 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 2 | 0.93 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 2 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 2 | 0.93 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 2 | 0.93 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 18 | 0.93 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 18 | 0.93 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 18 | 0.93 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 18 | 0.93 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 18 | 0.93 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 18 | 0.93 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 15 | 0.93 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 15 | 0.93 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 15 | 0.93 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 15 | 0.93 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 15 | 0.93 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 15 | 0.93 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 18 | 0.93 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 18 | 0.93 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 18 | 0.93 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 15 | 0.93 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 15 | 0.93 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 1 | 0.92 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 1 | 0.92 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 1 | 0.92 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 12 | 0.92 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 12 | 0.92 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 12 | 0.92 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 5 | 0.92 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 5 | 0.92 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 5 | 0.92 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 5 | 0.92 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 5 | 0.92 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 5 | 0.92 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 3 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 3 | 0.92 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 3 | 0.92 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG21 | 12 | 0.92 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG22 | 12 | 0.92 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG23 | 12 | 0.92 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 8 | 0.92 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 8 | 0.92 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 8 | 0.92 |
| (1,94) | 1:18:A:LEU:HA | 1:21:A:GLU:HB2 | 16 | 0.92 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD11 | 18 | 0.91 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD12 | 18 | 0.91 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD13 | 18 | 0.91 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 16 | 0.91 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 7 | 0.91 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 2 | 0.91 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 4 | 0.91 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 4 | 0.91 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 5 | 0.9 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 5 | 0.9 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 5 | 0.9 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG21 | 15 | 0.9 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG22 | 15 | 0.9 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG23 | 15 | 0.9 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 11 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 11 | 0.9 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 11 | 0.9 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 5 | 0.9 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 5 | 0.9 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 5 | 0.9 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 1 | 0.9 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 1 | 0.9 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 1 | 0.9 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 18 | 0.9 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 18 | 0.9 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 8 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 8 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 8 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 9 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 9 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 9 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 18 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 18 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 18 | 0.89 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 11 | 0.89 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 11 | 0.89 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 11 | 0.89 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 11 | 0.89 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 11 | 0.89 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 11 | 0.89 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 2 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 2 | 0.89 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 2 | 0.89 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 13 | 0.89 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 13 | 0.89 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 13 | 0.89 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 18 | 0.89 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 18 | 0.89 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 18 | 0.89 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 14 | 0.89 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 14 | 0.89 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 14 | 0.89 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 1 | 0.89 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 1 | 0.89 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 6 | 0.88 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 6 | 0.88 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 6 | 0.88 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 20 | 0.88 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 20 | 0.88 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 20 | 0.88 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 14 | 0.88 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 14 | 0.88 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 15 | 0.88 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 7 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 7 | 0.88 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 7 | 0.88 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 5 | 0.88 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 3 | 0.88 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 3 | 0.88 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 3 | 0.87 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 3 | 0.87 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 3 | 0.87 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 17 | 0.87 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 17 | 0.87 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 17 | 0.87 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 15 | 0.87 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 15 | 0.87 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 15 | 0.87 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 3 | 0.87 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 3 | 0.87 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 3 | 0.87 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 13 | 0.87 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 13 | 0.87 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 13 | 0.87 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 2 | 0.86 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 2 | 0.86 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 2 | 0.86 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 10 | 0.86 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 10 | 0.86 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 10 | 0.86 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 13 | 0.86 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 13 | 0.86 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 13 | 0.86 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 13 | 0.86 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 13 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 13 | 0.86 |
| (1,867) | 1:7:A:PRO:HA | 1:8:A:GLU:HB2 | 12 | 0.86 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 14 | 0.86 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 7 | 0.85 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 7 | 0.85 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 7 | 0.85 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 17 | 0.85 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 17 | 0.85 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 17 | 0.85 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 17 | 0.85 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 17 | 0.85 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 17 | 0.85 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG21 | 5 | 0.85 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG22 | 5 | 0.85 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG23 | 5 | 0.85 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 4 | 0.85 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 15 | 0.85 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 15 | 0.85 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 15 | 0.85 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 3 | 0.85 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 4 | 0.84 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 4 | 0.84 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 4 | 0.84 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 18 | 0.84 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 18 | 0.84 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 15 | 0.84 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 15 | 0.84 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 15 | 0.84 |
| (1,94) | 1:18:A:LEU:HA | 1:21:A:GLU:HB2 | 6 | 0.84 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG21 | 13 | 0.84 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG22 | 13 | 0.84 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG23 | 13 | 0.84 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 3 | 0.83 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 3 | 0.82 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 3 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 3 | 0.82 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 3 | 0.82 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 3 | 0.82 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 3 | 0.82 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 1 | 0.82 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 1 | 0.82 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 1 | 0.82 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 1 | 0.82 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 1 | 0.82 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 1 | 0.82 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 5 | 0.82 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 5 | 0.82 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 12 | 0.82 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 12 | 0.82 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 12 | 0.82 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 19 | 0.82 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 19 | 0.82 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 14 | 0.81 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 14 | 0.81 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 20 | 0.81 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 20 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 20 | 0.81 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD21 | 11 | 0.81 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD22 | 11 | 0.81 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD23 | 11 | 0.81 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 4 | 0.81 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 4 | 0.81 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 4 | 0.81 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 11 | 0.8 |
| (1,743) | 1:28:A:VAL:HG11 | 1:70:A:PRO:HB3 | 18 | 0.8 |
| (1,743) | 1:28:A:VAL:HG12 | 1:70:A:PRO:HB3 | 18 | 0.8 |
| (1,743) | 1:28:A:VAL:HG13 | 1:70:A:PRO:HB3 | 18 | 0.8 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 10 | 0.8 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 10 | 0.8 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 10 | 0.8 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 7 | 0.79 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 7 | 0.79 |
| (1,954) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 7 | 0.79 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 7 | 0.79 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 7 | 0.79 |
| (1,954) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 7 | 0.79 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 18 | 0.79 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 10 | 0.79 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 3 | 0.78 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 19 | 0.78 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 19 | 0.78 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 19 | 0.78 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 15 | 0.78 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 15 | 0.78 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD21 | 15 | 0.77 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD22 | 15 | 0.77 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD23 | 15 | 0.77 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD21 | 17 | 0.77 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD22 | 17 | 0.77 |
| (1,705) | 1:19:A:TYR:HE1 | 1:37:A:LEU:HD23 | 17 | 0.77 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD21 | 17 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD22 | 17 | 0.77 |
| (1,705) | 1:19:A:TYR:HE2 | 1:37:A:LEU:HD23 | 17 | 0.77 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 7 | 0.77 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 12 | 0.77 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 1 | 0.77 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 1 | 0.77 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 1 | 0.77 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 4 | 0.76 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 4 | 0.76 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD21 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD22 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD23 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD21 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD22 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD23 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD21 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD22 | 11 | 0.76 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD23 | 11 | 0.76 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 14 | 0.76 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 14 | 0.76 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 14 | 0.76 |
| (1,742) | 1:28:A:VAL:HG11 | 1:32:A:ASP:HB2 | 18 | 0.76 |
| (1,742) | 1:28:A:VAL:HG12 | 1:32:A:ASP:HB2 | 18 | 0.76 |
| (1,742) | 1:28:A:VAL:HG13 | 1:32:A:ASP:HB2 | 18 | 0.76 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 4 | 0.76 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 4 | 0.76 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 4 | 0.76 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 18 | 0.76 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 4 | 0.76 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 4 | 0.76 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 4 | 0.76 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 20 | 0.76 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 20 | 0.76 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 20 | 0.76 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 17 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 17 | 0.75 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 17 | 0.75 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 7 | 0.75 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 7 | 0.75 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 18 | 0.74 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 18 | 0.74 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 18 | 0.74 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 8 | 0.74 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 8 | 0.74 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 8 | 0.74 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 14 | 0.74 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 14 | 0.74 |
| (1,4) | 1:15:A:LEU:HD11 | 1:74:A:ALA:HA | 3 | 0.74 |
| (1,4) | 1:15:A:LEU:HD12 | 1:74:A:ALA:HA | 3 | 0.74 |
| (1,4) | 1:15:A:LEU:HD13 | 1:74:A:ALA:HA | 3 | 0.74 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 12 | 0.73 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 12 | 0.73 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 12 | 0.73 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 18 | 0.73 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 18 | 0.73 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 18 | 0.73 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 2 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 20 | 0.73 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 3 | 0.73 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD21 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD22 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD23 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD21 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD22 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD23 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD21 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD22 | 18 | 0.72 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD23 | 18 | 0.72 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 12 | 0.72 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 12 | 0.72 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 12 | 0.72 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 20 | 0.72 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 2 | 0.72 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 2 | 0.72 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 2 | 0.72 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 19 | 0.71 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 19 | 0.71 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 17 | 0.71 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 13 | 0.7 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 13 | 0.7 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 16 | 0.7 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 16 | 0.7 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 16 | 0.7 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 3 | 0.7 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 3 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 3 | 0.7 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 3 | 0.7 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 3 | 0.7 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 3 | 0.7 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD21 | 13 | 0.7 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD22 | 13 | 0.7 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD23 | 13 | 0.7 |
| (1,4) | 1:15:A:LEU:HD11 | 1:74:A:ALA:HA | 7 | 0.7 |
| (1,4) | 1:15:A:LEU:HD12 | 1:74:A:ALA:HA | 7 | 0.7 |
| (1,4) | 1:15:A:LEU:HD13 | 1:74:A:ALA:HA | 7 | 0.7 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD21 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD22 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD23 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD21 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD22 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD23 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD21 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD22 | 13 | 0.69 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD23 | 13 | 0.69 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 14 | 0.69 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 14 | 0.69 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 14 | 0.69 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 16 | 0.68 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 16 | 0.68 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 16 | 0.68 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 16 | 0.68 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 16 | 0.68 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 16 | 0.68 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG21 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG22 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG21 | 1:73:A:VAL:HG23 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG21 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG22 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG22 | 1:73:A:VAL:HG23 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG21 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG22 | 15 | 0.68 |
| (1,833) | 1:69:A:THR:HG23 | 1:73:A:VAL:HG23 | 15 | 0.68 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD21 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD22 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD23 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD21 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD22 | 12 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD23 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD21 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD22 | 12 | 0.68 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD23 | 12 | 0.68 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 18 | 0.68 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 18 | 0.68 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 18 | 0.68 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 18 | 0.68 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 18 | 0.68 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 18 | 0.68 |
| (1,4) | 1:15:A:LEU:HD11 | 1:74:A:ALA:HA | 18 | 0.68 |
| (1,4) | 1:15:A:LEU:HD12 | 1:74:A:ALA:HA | 18 | 0.68 |
| (1,4) | 1:15:A:LEU:HD13 | 1:74:A:ALA:HA | 18 | 0.68 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 2 | 0.67 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 2 | 0.67 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 2 | 0.67 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 2 | 0.67 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 2 | 0.67 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 2 | 0.67 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 2 | 0.67 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 2 | 0.67 |
| (1,718) | 1:75:A:ARG:HA | 1:75:A:ARG:HD3 | 14 | 0.67 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 20 | 0.67 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 13 | 0.67 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 10 | 0.67 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 10 | 0.67 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 10 | 0.67 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 10 | 0.67 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 10 | 0.67 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 10 | 0.67 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 2 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 2 | 0.67 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 2 | 0.67 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 13 | 0.66 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 13 | 0.66 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 1 | 0.66 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 10 | 0.66 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 10 | 0.66 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 2 | 0.65 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 2 | 0.65 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 10 | 0.65 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 10 | 0.65 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 1 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 1 | 0.65 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 1 | 0.65 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 1 | 0.65 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 1 | 0.65 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 1 | 0.65 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 14 | 0.65 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 14 | 0.65 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 14 | 0.65 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 14 | 0.65 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 14 | 0.65 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 14 | 0.65 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG21 | 11 | 0.65 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG22 | 11 | 0.65 |
| (1,772) | 1:55:A:LEU:HB2 | 1:57:A:VAL:HG23 | 11 | 0.65 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 19 | 0.65 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 19 | 0.65 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 19 | 0.65 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 19 | 0.65 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 6 | 0.65 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 6 | 0.65 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 6 | 0.65 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 15 | 0.64 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 15 | 0.64 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 15 | 0.64 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 15 | 0.64 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 15 | 0.64 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 15 | 0.64 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 12 | 0.64 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 12 | 0.64 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 12 | 0.64 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 18 | 0.64 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 18 | 0.64 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 18 | 0.64 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 12 | 0.64 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 12 | 0.64 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 12 | 0.64 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 3 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 3 | 0.63 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 3 | 0.63 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 9 | 0.63 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 3 | 0.63 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 9 | 0.63 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 15 | 0.63 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 1 | 0.63 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 14 | 0.63 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 1 | 0.62 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 1 | 0.62 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 9 | 0.62 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 9 | 0.62 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 9 | 0.62 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 10 | 0.62 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 10 | 0.62 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 10 | 0.62 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 4 | 0.62 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 4 | 0.62 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 4 | 0.62 |
| (1,717) | 1:28:A:VAL:HG11 | 1:32:A:ASP:HB3 | 18 | 0.62 |
| (1,717) | 1:28:A:VAL:HG12 | 1:32:A:ASP:HB3 | 18 | 0.62 |
| (1,717) | 1:28:A:VAL:HG13 | 1:32:A:ASP:HB3 | 18 | 0.62 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 17 | 0.62 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 10 | 0.62 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD11 | 2 | 0.62 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD12 | 2 | 0.62 |
| (1,475) | 1:74:A:ALA:H | 1:77:A:LEU:HD13 | 2 | 0.62 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 9 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 9 | 0.62 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 9 | 0.62 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 12 | 0.62 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 12 | 0.62 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 12 | 0.62 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG11 | 13 | 0.61 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG12 | 13 | 0.61 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG13 | 13 | 0.61 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG11 | 13 | 0.61 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG12 | 13 | 0.61 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG13 | 13 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 16 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 16 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 16 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 20 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 20 | 0.61 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 20 | 0.61 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 10 | 0.61 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 10 | 0.61 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 10 | 0.61 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 10 | 0.61 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 10 | 0.61 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 10 | 0.61 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 14 | 0.61 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 14 | 0.61 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 14 | 0.61 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 17 | 0.61 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 3 | 0.61 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 3 | 0.61 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 3 | 0.61 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 18 | 0.61 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 18 | 0.61 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 18 | 0.61 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 4 | 0.61 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG11 | 18 | 0.6 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG12 | 18 | 0.6 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG13 | 18 | 0.6 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG11 | 18 | 0.6 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG12 | 18 | 0.6 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG13 | 18 | 0.6 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 9 | 0.6 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 9 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 9 | 0.6 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 4 | 0.6 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 4 | 0.6 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 4 | 0.6 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 11 | 0.6 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 11 | 0.6 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 11 | 0.6 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 13 | 0.59 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 13 | 0.59 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 3 | 0.59 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 3 | 0.59 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 3 | 0.59 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 12 | 0.59 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 12 | 0.59 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 12 | 0.59 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 20 | 0.59 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 20 | 0.59 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 20 | 0.59 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 19 | 0.59 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 19 | 0.59 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 6 | 0.59 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 13 | 0.59 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 15 | 0.59 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 16 | 0.59 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 16 | 0.59 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 16 | 0.59 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 5 | 0.59 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 5 | 0.59 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 5 | 0.59 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 5 | 0.59 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 5 | 0.59 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 5 | 0.59 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 5 | 0.59 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 5 | 0.59 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 5 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 7 | 0.59 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 7 | 0.59 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 7 | 0.59 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 10 | 0.58 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 10 | 0.58 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 15 | 0.58 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 15 | 0.58 |
| (1,743) | 1:28:A:VAL:HG11 | 1:70:A:PRO:HB3 | 13 | 0.58 |
| (1,743) | 1:28:A:VAL:HG12 | 1:70:A:PRO:HB3 | 13 | 0.58 |
| (1,743) | 1:28:A:VAL:HG13 | 1:70:A:PRO:HB3 | 13 | 0.58 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 15 | 0.58 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 15 | 0.58 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 15 | 0.58 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 15 | 0.58 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 15 | 0.58 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 15 | 0.58 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 7 | 0.58 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 12 | 0.58 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 12 | 0.58 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 12 | 0.58 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 17 | 0.58 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 17 | 0.58 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 17 | 0.58 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 2 | 0.58 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 2 | 0.58 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 2 | 0.58 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 7 | 0.57 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 7 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 7 | 0.57 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 20 | 0.57 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 20 | 0.57 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 20 | 0.57 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 19 | 0.57 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 19 | 0.57 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 19 | 0.57 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 16 | 0.57 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 16 | 0.57 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 16 | 0.57 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 16 | 0.57 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 14 | 0.57 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 14 | 0.57 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 4 | 0.56 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 14 | 0.56 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 14 | 0.56 |
| (1,910) | 1:75:A:ARG:HG3 | 1:76:A:ALA:H | 15 | 0.56 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 5 | 0.56 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 5 | 0.56 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 5 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 18 | 0.56 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 18 | 0.56 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 18 | 0.56 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 5 | 0.56 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 16 | 0.56 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 16 | 0.56 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 15 | 0.56 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 15 | 0.56 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 15 | 0.56 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 19 | 0.56 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 19 | 0.56 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 19 | 0.56 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 12 | 0.55 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 12 | 0.55 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 5 | 0.55 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 5 | 0.55 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG11 | 11 | 0.55 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG12 | 11 | 0.55 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG13 | 11 | 0.55 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG11 | 11 | 0.55 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG12 | 11 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG13 | 11 | 0.55 |
| (1,910) | 1:75:A:ARG:HG3 | 1:76:A:ALA:H | 20 | 0.55 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 15 | 0.55 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 15 | 0.55 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 15 | 0.55 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 1 | 0.55 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 11 | 0.55 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 6 | 0.55 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 8 | 0.55 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 14 | 0.55 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 14 | 0.55 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 14 | 0.55 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 18 | 0.55 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 18 | 0.55 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 18 | 0.55 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 11 | 0.55 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 11 | 0.55 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 11 | 0.55 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 20 | 0.55 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 20 | 0.55 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 20 | 0.55 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 15 | 0.54 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 15 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 13 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 20 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 20 | 0.54 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 20 | 0.54 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG21 | 18 | 0.54 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG22 | 18 | 0.54 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG23 | 18 | 0.54 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 3 | 0.54 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 3 | 0.54 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 3 | 0.54 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 5 | 0.54 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 5 | 0.54 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 5 | 0.54 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 5 | 0.54 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 5 | 0.54 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 5 | 0.54 |
| (1,576) | 1:12:A:GLU:H | 1:13:A:LYS:HG3 | 20 | 0.54 |
| (1,195) | 1:13:A:LYS:HG3 | 1:14:A:VAL:H | 16 | 0.54 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG11 | 12 | 0.54 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG12 | 12 | 0.54 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG13 | 12 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 3 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 3 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 3 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 6 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 6 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 6 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 18 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 18 | 0.54 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 18 | 0.54 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 4 | 0.54 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 4 | 0.54 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 4 | 0.54 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 17 | 0.54 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 17 | 0.54 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 17 | 0.54 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 5 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 5 | 0.53 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 20 | 0.53 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 20 | 0.53 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 18 | 0.53 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 18 | 0.53 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD21 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD22 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG11 | 1:37:A:LEU:HD23 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD21 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD22 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG12 | 1:37:A:LEU:HD23 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD21 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD22 | 14 | 0.53 |
| (1,830) | 1:28:A:VAL:HG13 | 1:37:A:LEU:HD23 | 14 | 0.53 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 3 | 0.53 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 3 | 0.53 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 3 | 0.53 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 7 | 0.53 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 7 | 0.53 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 7 | 0.53 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 9 | 0.53 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 9 | 0.53 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 9 | 0.53 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 12 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 12 | 0.53 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 12 | 0.53 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 5 | 0.53 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 5 | 0.53 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 5 | 0.53 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 5 | 0.53 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 5 | 0.53 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 5 | 0.53 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 12 | 0.53 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 18 | 0.53 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 17 | 0.53 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 20 | 0.53 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 20 | 0.53 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 20 | 0.53 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 18 | 0.53 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 18 | 0.53 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 18 | 0.53 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD11 | 15 | 0.53 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD12 | 15 | 0.53 |
| (1,114) | 1:61:A:ILE:HG13 | 1:64:A:LEU:HD13 | 15 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 4 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 4 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 4 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 13 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 13 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 13 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 16 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 16 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 16 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 17 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 17 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 17 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 20 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 20 | 0.53 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 20 | 0.53 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 3 | 0.53 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 3 | 0.53 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 3 | 0.53 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD21 | 15 | 0.52 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD22 | 15 | 0.52 |
| (1,851) | 1:43:A:LEU:HA | 1:43:A:LEU:HD23 | 15 | 0.52 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 11 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 11 | 0.52 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 11 | 0.52 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 20 | 0.52 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 20 | 0.52 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 20 | 0.52 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 1 | 0.52 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 10 | 0.52 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 9 | 0.52 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 9 | 0.52 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 9 | 0.52 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 16 | 0.52 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 16 | 0.52 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 16 | 0.52 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 18 | 0.52 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 3 | 0.52 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 3 | 0.52 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 3 | 0.52 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 1 | 0.52 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 1 | 0.52 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 1 | 0.52 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 7 | 0.52 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 7 | 0.52 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 7 | 0.52 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 2 | 0.52 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 2 | 0.52 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 2 | 0.52 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 3 | 0.51 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 3 | 0.51 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG11 | 12 | 0.51 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG12 | 12 | 0.51 |
| (1,963) | 1:19:A:TYR:HD1 | 1:28:A:VAL:HG13 | 12 | 0.51 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG11 | 12 | 0.51 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG12 | 12 | 0.51 |
| (1,963) | 1:19:A:TYR:HD2 | 1:28:A:VAL:HG13 | 12 | 0.51 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 3 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 3 | 0.51 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 3 | 0.51 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 3 | 0.51 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 3 | 0.51 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 3 | 0.51 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 11 | 0.51 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 11 | 0.51 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 11 | 0.51 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD21 | 8 | 0.51 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD22 | 8 | 0.51 |
| (1,723) | 1:18:A:LEU:HB2 | 1:47:A:LEU:HD23 | 8 | 0.51 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 12 | 0.51 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 12 | 0.51 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 12 | 0.51 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 18 | 0.51 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG21 | 18 | 0.51 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG22 | 18 | 0.51 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG23 | 18 | 0.51 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 9 | 0.51 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 9 | 0.51 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 9 | 0.51 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 3 | 0.51 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 3 | 0.51 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 15 | 0.51 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 15 | 0.51 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 15 | 0.51 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 13 | 0.51 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 13 | 0.51 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 7 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 7 | 0.51 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 7 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 8 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 8 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 8 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 9 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 9 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 9 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 10 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 10 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 10 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 12 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 12 | 0.51 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 12 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 5 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 5 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 5 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 18 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 18 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 18 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 19 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 19 | 0.51 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 19 | 0.51 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 20 | 0.51 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 20 | 0.51 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 20 | 0.51 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 4 | 0.5 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 4 | 0.5 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 4 | 0.5 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 18 | 0.5 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 18 | 0.5 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 18 | 0.5 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 18 | 0.5 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 18 | 0.5 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 18 | 0.5 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 4 | 0.5 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 4 | 0.5 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 4 | 0.5 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 7 | 0.5 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 7 | 0.5 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 7 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 8 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 8 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 8 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 14 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 14 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 14 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 20 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 20 | 0.5 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 20 | 0.5 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 16 | 0.5 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 16 | 0.5 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 16 | 0.5 |
| (1,717) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 13 | 0.5 |
| (1,717) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 13 | 0.5 |
| (1,717) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 13 | 0.5 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 8 | 0.5 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 13 | 0.5 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 13 | 0.5 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 13 | 0.5 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 14 | 0.5 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 14 | 0.5 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 14 | 0.5 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 15 | 0.5 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 14 | 0.5 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 14 | 0.5 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 14 | 0.5 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 16 | 0.5 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 16 | 0.5 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 16 | 0.5 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD11 | 14 | 0.5 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD12 | 14 | 0.5 |
| (1,10) | 1:23:A:LEU:HA | 1:23:A:LEU:HD13 | 14 | 0.5 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 16 | 0.5 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 16 | 0.5 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 16 | 0.5 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 6 | 0.49 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 6 | 0.49 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 6 | 0.49 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 16 | 0.49 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 16 | 0.49 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 16 | 0.49 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 10 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 10 | 0.49 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 10 | 0.49 |
| (1,910) | 1:75:A:ARG:HG3 | 1:76:A:ALA:H | 9 | 0.49 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 19 | 0.49 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 19 | 0.49 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 19 | 0.49 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 4 | 0.49 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 19 | 0.49 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 19 | 0.49 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 19 | 0.49 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 19 | 0.49 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 3 | 0.49 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 14 | 0.49 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 19 | 0.49 |
| (1,110) | 1:62:A:ARG:HA | 1:62:A:ARG:HD2 | 4 | 0.49 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 18 | 0.48 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 18 | 0.48 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 18 | 0.48 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 19 | 0.48 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 19 | 0.48 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 19 | 0.48 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 7 | 0.48 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 19 | 0.48 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 19 | 0.48 |
| (1,731) | 1:51:A:ILE:HG21 | 1:52:A:ARG:HG3 | 20 | 0.48 |
| (1,731) | 1:51:A:ILE:HG22 | 1:52:A:ARG:HG3 | 20 | 0.48 |
| (1,731) | 1:51:A:ILE:HG23 | 1:52:A:ARG:HG3 | 20 | 0.48 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 14 | 0.48 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 14 | 0.48 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 14 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 16 | 0.48 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 16 | 0.48 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 16 | 0.48 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 5 | 0.48 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 12 | 0.48 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 12 | 0.48 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 12 | 0.48 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 16 | 0.48 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 16 | 0.48 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 16 | 0.48 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 20 | 0.48 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 7 | 0.48 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 20 | 0.48 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 8 | 0.48 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 8 | 0.48 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 8 | 0.48 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 14 | 0.48 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD21 | 11 | 0.48 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD22 | 11 | 0.48 |
| (1,5) | 1:18:A:LEU:HA | 1:18:A:LEU:HD23 | 11 | 0.48 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 20 | 0.47 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 20 | 0.47 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 20 | 0.47 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 9 | 0.47 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 9 | 0.47 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 9 | 0.47 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 13 | 0.47 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 13 | 0.47 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 13 | 0.47 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 5 | 0.47 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 5 | 0.47 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 5 | 0.47 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 17 | 0.47 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 17 | 0.47 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 17 | 0.47 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 3 | 0.47 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 3 | 0.47 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 3 | 0.47 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 10 | 0.47 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 10 | 0.47 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 10 | 0.47 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 2 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 2 | 0.47 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 2 | 0.47 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 1 | 0.47 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 4 | 0.47 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 4 | 0.47 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 4 | 0.47 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 10 | 0.47 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 10 | 0.47 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 10 | 0.47 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 8 | 0.46 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 8 | 0.46 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 8 | 0.46 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 10 | 0.46 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 10 | 0.46 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 10 | 0.46 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 19 | 0.46 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 19 | 0.46 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 20 | 0.46 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 20 | 0.46 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 3 | 0.46 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 3 | 0.46 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 3 | 0.46 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 3 | 0.46 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 3 | 0.46 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 3 | 0.46 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 8 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 8 | 0.46 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 8 | 0.46 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 16 | 0.46 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 16 | 0.46 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 16 | 0.46 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 20 | 0.46 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 20 | 0.46 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 20 | 0.46 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 3 | 0.46 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG21 | 12 | 0.46 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG22 | 12 | 0.46 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG23 | 12 | 0.46 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 18 | 0.46 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 18 | 0.46 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 18 | 0.46 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 17 | 0.46 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 12 | 0.46 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 3 | 0.46 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 3 | 0.46 |
| (1,1046) | 1:59:A:LEU:HD11 | 1:64:A:LEU:HD11 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD11 | 1:64:A:LEU:HD12 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD11 | 1:64:A:LEU:HD13 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD12 | 1:64:A:LEU:HD11 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD12 | 1:64:A:LEU:HD12 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD12 | 1:64:A:LEU:HD13 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD13 | 1:64:A:LEU:HD11 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD13 | 1:64:A:LEU:HD12 | 10 | 0.45 |
| (1,1046) | 1:59:A:LEU:HD13 | 1:64:A:LEU:HD13 | 10 | 0.45 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 6 | 0.45 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 6 | 0.45 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 2 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 2 | 0.45 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 2 | 0.45 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 4 | 0.45 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 4 | 0.45 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 4 | 0.45 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 2 | 0.45 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 2 | 0.45 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 2 | 0.45 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 17 | 0.45 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 17 | 0.45 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 17 | 0.45 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 18 | 0.45 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 18 | 0.45 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 18 | 0.45 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 3 | 0.45 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 3 | 0.45 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 3 | 0.45 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 7 | 0.45 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 7 | 0.45 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 7 | 0.45 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 8 | 0.45 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 8 | 0.45 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 8 | 0.45 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 18 | 0.45 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 18 | 0.45 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 18 | 0.45 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 18 | 0.45 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 18 | 0.45 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 18 | 0.45 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 18 | 0.45 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 18 | 0.45 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 18 | 0.45 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 8 | 0.45 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 8 | 0.45 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 8 | 0.45 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 12 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 12 | 0.44 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 12 | 0.44 |
| (1,869) | 1:46:A:ARG:HA | 1:46:A:ARG:HD2 | 6 | 0.44 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 8 | 0.44 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 8 | 0.44 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 8 | 0.44 |
| (1,643) | 1:21:A:GLU:H | 1:22:A:ILE:HG13 | 7 | 0.44 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 5 | 0.44 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG21 | 16 | 0.44 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG22 | 16 | 0.44 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG23 | 16 | 0.44 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 6 | 0.44 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 6 | 0.44 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 6 | 0.44 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 13 | 0.44 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 1 | 0.44 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 1 | 0.44 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 1 | 0.44 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 3 | 0.44 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 13 | 0.44 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 18 | 0.44 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 18 | 0.44 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 16 | 0.44 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 16 | 0.44 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 16 | 0.44 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 3 | 0.44 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 3 | 0.44 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 3 | 0.44 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 6 | 0.44 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 6 | 0.44 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 6 | 0.44 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 8 | 0.43 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 8 | 0.43 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 8 | 0.43 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 8 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 8 | 0.43 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 8 | 0.43 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 12 | 0.43 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 12 | 0.43 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 12 | 0.43 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 12 | 0.43 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 12 | 0.43 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 12 | 0.43 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 1 | 0.43 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 1 | 0.43 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 20 | 0.43 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 20 | 0.43 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 20 | 0.43 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 11 | 0.43 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 1 | 0.43 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 1 | 0.43 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 1 | 0.43 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 5 | 0.43 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 5 | 0.43 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 5 | 0.43 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 13 | 0.43 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 13 | 0.43 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 13 | 0.43 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 18 | 0.43 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 18 | 0.43 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 18 | 0.43 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 3 | 0.43 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 3 | 0.43 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 3 | 0.43 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 4 | 0.43 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 5 | 0.43 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 11 | 0.43 |
| (1,195) | 1:13:A:LYS:HG3 | 1:14:A:VAL:H | 10 | 0.43 |
| (1,195) | 1:13:A:LYS:HG3 | 1:14:A:VAL:H | 17 | 0.43 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 5 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 5 | 0.43 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 5 | 0.43 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 4 | 0.43 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 4 | 0.43 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 4 | 0.43 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 20 | 0.43 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 20 | 0.43 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 20 | 0.43 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 20 | 0.43 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 20 | 0.43 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 20 | 0.43 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 10 | 0.43 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 10 | 0.43 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 10 | 0.43 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD11 | 15 | 0.42 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD12 | 15 | 0.42 |
| (1,1020) | 1:55:A:LEU:HA | 1:55:A:LEU:HD13 | 15 | 0.42 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 2 | 0.42 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 2 | 0.42 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 2 | 0.42 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 2 | 0.42 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 2 | 0.42 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 2 | 0.42 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 13 | 0.42 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 13 | 0.42 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 13 | 0.42 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 12 | 0.42 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 15 | 0.42 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 15 | 0.42 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 15 | 0.42 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 12 | 0.42 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 12 | 0.42 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 12 | 0.42 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG21 | 14 | 0.42 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG22 | 14 | 0.42 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG23 | 14 | 0.42 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 6 | 0.42 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 11 | 0.42 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 5 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 5 | 0.42 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 5 | 0.42 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 19 | 0.42 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 19 | 0.42 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 19 | 0.42 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 14 | 0.42 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 14 | 0.42 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 14 | 0.42 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 18 | 0.41 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 18 | 0.41 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 18 | 0.41 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 19 | 0.41 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 19 | 0.41 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 20 | 0.41 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 20 | 0.41 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 20 | 0.41 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 7 | 0.41 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 7 | 0.41 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 7 | 0.41 |
| (1,743) | 1:28:A:VAL:HG11 | 1:70:A:PRO:HB3 | 12 | 0.41 |
| (1,743) | 1:28:A:VAL:HG12 | 1:70:A:PRO:HB3 | 12 | 0.41 |
| (1,743) | 1:28:A:VAL:HG13 | 1:70:A:PRO:HB3 | 12 | 0.41 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 18 | 0.41 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 18 | 0.41 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 18 | 0.41 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 7 | 0.41 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 7 | 0.41 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 7 | 0.41 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 14 | 0.41 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 11 | 0.41 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 11 | 0.41 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 19 | 0.41 |
| (1,246) | 1:21:A:GLU:HG2 | 1:22:A:ILE:H | 19 | 0.41 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 20 | 0.41 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 20 | 0.41 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 20 | 0.41 |
| (1,110) | 1:62:A:ARG:HA | 1:62:A:ARG:HD2 | 7 | 0.41 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 6 | 0.41 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 6 | 0.41 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 1 | 0.41 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 1 | 0.41 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 1 | 0.41 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 14 | 0.41 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 14 | 0.41 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 14 | 0.41 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 4 | 0.4 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 4 | 0.4 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 4 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 10 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 10 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 10 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 20 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 20 | 0.4 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 20 | 0.4 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 13 | 0.4 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 13 | 0.4 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 7 | 0.4 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 7 | 0.4 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 7 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 13 | 0.4 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 13 | 0.4 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 13 | 0.4 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 20 | 0.4 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 1 | 0.4 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 1 | 0.4 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 1 | 0.4 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 2 | 0.4 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 2 | 0.4 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 2 | 0.4 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 7 | 0.4 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 7 | 0.4 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 7 | 0.4 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 7 | 0.4 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 2 | 0.4 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 9 | 0.4 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 4 | 0.4 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 4 | 0.4 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 4 | 0.4 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 16 | 0.4 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 16 | 0.4 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 16 | 0.4 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 20 | 0.4 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 20 | 0.4 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 2 | 0.4 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 2 | 0.4 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 2 | 0.4 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 15 | 0.4 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 15 | 0.4 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 15 | 0.4 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 9 | 0.4 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 9 | 0.4 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 9 | 0.4 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 1 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 1 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 1 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 3 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 3 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 3 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 10 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 10 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 10 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 14 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 14 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 14 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 15 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 15 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 15 | 0.39 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 12 | 0.39 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 12 | 0.39 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 12 | 0.39 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 8 | 0.39 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 11 | 0.39 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 11 | 0.39 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 17 | 0.39 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 17 | 0.39 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 17 | 0.39 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 17 | 0.39 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 17 | 0.39 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 17 | 0.39 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD11 | 3 | 0.39 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD12 | 3 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD13 | 3 | 0.39 |
| (1,853) | 1:91:A:LYS:HA | 1:91:A:LYS:HD3 | 16 | 0.39 |
| (1,803) | 1:59:A:LEU:HD21 | 1:73:A:VAL:HG21 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD21 | 1:73:A:VAL:HG22 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD21 | 1:73:A:VAL:HG23 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD22 | 1:73:A:VAL:HG21 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD22 | 1:73:A:VAL:HG22 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD22 | 1:73:A:VAL:HG23 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD23 | 1:73:A:VAL:HG21 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD23 | 1:73:A:VAL:HG22 | 4 | 0.39 |
| (1,803) | 1:59:A:LEU:HD23 | 1:73:A:VAL:HG23 | 4 | 0.39 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 3 | 0.39 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 3 | 0.39 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 3 | 0.39 |
| (1,725) | 1:44:A:ALA:HB1 | 1:45:A:MET:HB3 | 6 | 0.39 |
| (1,725) | 1:44:A:ALA:HB2 | 1:45:A:MET:HB3 | 6 | 0.39 |
| (1,725) | 1:44:A:ALA:HB3 | 1:45:A:MET:HB3 | 6 | 0.39 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 4 | 0.39 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 4 | 0.39 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 4 | 0.39 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG21 | 13 | 0.39 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG22 | 13 | 0.39 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG23 | 13 | 0.39 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 19 | 0.39 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 9 | 0.39 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 4 | 0.39 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 4 | 0.39 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 4 | 0.39 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 10 | 0.39 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 10 | 0.39 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 10 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 5 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 5 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 5 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 17 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 17 | 0.39 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 17 | 0.39 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 6 | 0.39 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 6 | 0.39 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 6 | 0.39 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 13 | 0.38 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 13 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 13 | 0.38 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 18 | 0.38 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 18 | 0.38 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 12 | 0.38 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 12 | 0.38 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD21 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD22 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD21 | 1:64:A:LEU:HD23 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD21 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD22 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD22 | 1:64:A:LEU:HD23 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD21 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD22 | 6 | 0.38 |
| (1,750) | 1:59:A:LEU:HD23 | 1:64:A:LEU:HD23 | 6 | 0.38 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 16 | 0.38 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 16 | 0.38 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 16 | 0.38 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 3 | 0.38 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 3 | 0.38 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 3 | 0.38 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 10 | 0.38 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 19 | 0.38 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 19 | 0.38 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 19 | 0.38 |
| (1,322) | 1:46:A:ARG:HD2 | 1:47:A:LEU:H | 16 | 0.38 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 2 | 0.38 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 2 | 0.38 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 2 | 0.38 |
| (1,110) | 1:62:A:ARG:HA | 1:62:A:ARG:HD3 | 15 | 0.38 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 1 | 0.38 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 12 | 0.38 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 17 | 0.38 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 17 | 0.38 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 3 | 0.38 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 3 | 0.38 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 3 | 0.38 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 6 | 0.38 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 6 | 0.38 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 6 | 0.38 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 9 | 0.38 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 9 | 0.38 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 9 | 0.38 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 10 | 0.38 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 10 | 0.38 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 10 | 0.38 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG21 | 18 | 0.38 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG22 | 18 | 0.38 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG23 | 18 | 0.38 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 15 | 0.38 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 15 | 0.38 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 15 | 0.38 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 2 | 0.37 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 2 | 0.37 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 2 | 0.37 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 13 | 0.37 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 13 | 0.37 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 13 | 0.37 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 13 | 0.37 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 13 | 0.37 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 13 | 0.37 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 14 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 14 | 0.37 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 14 | 0.37 |
| (1,869) | 1:46:A:ARG:HA | 1:46:A:ARG:HD2 | 9 | 0.37 |
| (1,853) | 1:91:A:LYS:HA | 1:91:A:LYS:HD3 | 18 | 0.37 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD21 | 2 | 0.37 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD22 | 2 | 0.37 |
| (1,788) | 1:19:A:TYR:HB2 | 1:37:A:LEU:HD23 | 2 | 0.37 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 2 | 0.37 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 2 | 0.37 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 2 | 0.37 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 4 | 0.37 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 8 | 0.37 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 8 | 0.37 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 8 | 0.37 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 11 | 0.37 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 11 | 0.37 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 11 | 0.37 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 16 | 0.37 |
| (1,195) | 1:13:A:LYS:HG3 | 1:14:A:VAL:H | 1 | 0.37 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 18 | 0.37 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 18 | 0.37 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 18 | 0.37 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 7 | 0.37 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 7 | 0.37 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 7 | 0.37 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 7 | 0.37 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 9 | 0.37 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 9 | 0.37 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 9 | 0.37 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 13 | 0.37 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 13 | 0.37 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 13 | 0.37 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 5 | 0.36 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 5 | 0.36 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 5 | 0.36 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 6 | 0.36 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 6 | 0.36 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 6 | 0.36 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 6 | 0.36 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 6 | 0.36 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 6 | 0.36 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 12 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 12 | 0.36 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 12 | 0.36 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 8 | 0.36 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 8 | 0.36 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 8 | 0.36 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 14 | 0.36 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 14 | 0.36 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 9 | 0.36 |
| (1,627) | 1:54:A:GLU:H | 1:54:A:GLU:HG2 | 13 | 0.36 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 1 | 0.36 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 6 | 0.36 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 6 | 0.36 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 6 | 0.36 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 13 | 0.36 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 13 | 0.36 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 13 | 0.36 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 19 | 0.36 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 19 | 0.36 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 19 | 0.36 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 17 | 0.36 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 9 | 0.36 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 1 | 0.36 |
| (1,246) | 1:21:A:GLU:HG2 | 1:22:A:ILE:H | 9 | 0.36 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG21 | 11 | 0.36 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG22 | 11 | 0.36 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG23 | 11 | 0.36 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 16 | 0.36 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 16 | 0.36 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 16 | 0.36 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 14 | 0.36 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 14 | 0.36 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 14 | 0.36 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 11 | 0.36 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 11 | 0.36 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 8 | 0.36 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 8 | 0.36 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 8 | 0.36 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 6 | 0.36 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 6 | 0.36 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 6 | 0.36 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 5 | 0.35 |
| (1,993) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 5 | 0.35 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG21 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG22 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG23 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG21 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG22 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG23 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG21 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG22 | 1 | 0.35 |
| (1,991) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG23 | 1 | 0.35 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 11 | 0.35 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 11 | 0.35 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 11 | 0.35 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 14 | 0.35 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 14 | 0.35 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 14 | 0.35 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 19 | 0.35 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 19 | 0.35 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 19 | 0.35 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 1 | 0.35 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 1 | 0.35 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 1 | 0.35 |
| (1,628) | 1:53:A:GLU:HG3 | 1:54:A:GLU:H | 10 | 0.35 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 20 | 0.35 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 20 | 0.35 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 20 | 0.35 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 16 | 0.35 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 16 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 16 | 0.35 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 1 | 0.35 |
| (1,491) | 1:74:A:ALA:H | 1:75:A:ARG:HG3 | 12 | 0.35 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 19 | 0.35 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 19 | 0.35 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 19 | 0.35 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 10 | 0.35 |
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 2 | 0.35 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 13 | 0.35 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 13 | 0.35 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 13 | 0.35 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 2 | 0.35 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 9 | 0.35 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 9 | 0.35 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 10 | 0.35 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 10 | 0.35 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 10 | 0.35 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 7 | 0.35 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 7 | 0.35 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 7 | 0.35 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 19 | 0.34 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 19 | 0.34 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 19 | 0.34 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 5 | 0.34 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 5 | 0.34 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 5 | 0.34 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 5 | 0.34 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 5 | 0.34 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 5 | 0.34 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 20 | 0.34 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 20 | 0.34 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 20 | 0.34 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 20 | 0.34 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 20 | 0.34 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 20 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 16 | 0.34 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 16 | 0.34 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 16 | 0.34 |
| (1,924) | 1:62:A:ARG:HB3 | 1:63:A:GLN:HE21 | 7 | 0.34 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 15 | 0.34 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 15 | 0.34 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 15 | 0.34 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 15 | 0.34 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 15 | 0.34 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 15 | 0.34 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD11 | 19 | 0.34 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD12 | 19 | 0.34 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD13 | 19 | 0.34 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 1 | 0.34 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 1 | 0.34 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 1 | 0.34 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 20 | 0.34 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 20 | 0.34 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 20 | 0.34 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 11 | 0.34 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 14 | 0.34 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 7 | 0.34 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 7 | 0.34 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 7 | 0.34 |
| (1,195) | 1:13:A:LYS:HG3 | 1:14:A:VAL:H | 11 | 0.34 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 4 | 0.34 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 4 | 0.34 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 4 | 0.34 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 12 | 0.34 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 12 | 0.34 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 12 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 3 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 3 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 3 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 5 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 5 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 5 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 7 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 7 | 0.34 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 7 | 0.34 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 12 | 0.34 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 12 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 12 | 0.34 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD21 | 1 | 0.34 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD22 | 1 | 0.34 |
| (1,3) | 1:77:A:LEU:HA | 1:77:A:LEU:HD23 | 1 | 0.34 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD21 | 14 | 0.33 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD22 | 14 | 0.33 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD23 | 14 | 0.33 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 12 | 0.33 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 12 | 0.33 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 12 | 0.33 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 6 | 0.33 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 13 | 0.33 |
| (1,576) | 1:12:A:GLU:H | 1:13:A:LYS:HG3 | 10 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 3 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 3 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 3 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 8 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 8 | 0.33 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 8 | 0.33 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 15 | 0.33 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 16 | 0.33 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 10 | 0.33 |
| (1,400) | 1:55:A:LEU:HD11 | 1:56:A:GLY:H | 17 | 0.33 |
| (1,400) | 1:55:A:LEU:HD12 | 1:56:A:GLY:H | 17 | 0.33 |
| (1,400) | 1:55:A:LEU:HD13 | 1:56:A:GLY:H | 17 | 0.33 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 19 | 0.33 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 8 | 0.33 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 17 | 0.33 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 17 | 0.33 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 17 | 0.33 |
| (1,256) | 1:20:A:ALA:H | 1:28:A:VAL:HG21 | 18 | 0.33 |
| (1,256) | 1:20:A:ALA:H | 1:28:A:VAL:HG22 | 18 | 0.33 |
| (1,256) | 1:20:A:ALA:H | 1:28:A:VAL:HG23 | 18 | 0.33 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 6 | 0.33 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 6 | 0.33 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 6 | 0.33 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 19 | 0.33 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 19 | 0.33 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 19 | 0.33 |
| (1,110) | 1:62:A:ARG:HA | 1:62:A:ARG:HD2 | 8 | 0.33 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 10 | 0.33 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 19 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 19 | 0.33 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 19 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 3 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 3 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 3 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 13 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 13 | 0.33 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 13 | 0.33 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD11 | 7 | 0.32 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD12 | 7 | 0.32 |
| (1,900) | 1:12:A:GLU:H | 1:15:A:LEU:HD13 | 7 | 0.32 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 18 | 0.32 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 18 | 0.32 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 10 | 0.32 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 10 | 0.32 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 10 | 0.32 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 5 | 0.32 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 5 | 0.32 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 5 | 0.32 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 14 | 0.32 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 14 | 0.32 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 14 | 0.32 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 18 | 0.32 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 18 | 0.32 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 18 | 0.32 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 6 | 0.32 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 6 | 0.32 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 6 | 0.32 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 6 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 10 | 0.32 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 10 | 0.32 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 10 | 0.32 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 11 | 0.32 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 11 | 0.32 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 11 | 0.32 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 12 | 0.32 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 18 | 0.32 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 8 | 0.32 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 20 | 0.32 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 19 | 0.32 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 19 | 0.32 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 19 | 0.32 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 19 | 0.32 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 19 | 0.32 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 19 | 0.32 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 1 | 0.32 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 16 | 0.32 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 16 | 0.32 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 16 | 0.32 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 17 | 0.32 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 17 | 0.32 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 17 | 0.32 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 16 | 0.31 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 11 | 0.31 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 11 | 0.31 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 11 | 0.31 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 7 | 0.31 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 7 | 0.31 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 7 | 0.31 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 7 | 0.31 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 7 | 0.31 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 7 | 0.31 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 1 | 0.31 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 1 | 0.31 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 1 | 0.31 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 12 | 0.31 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 12 | 0.31 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 12 | 0.31 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 1 | 0.31 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 1 | 0.31 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 1 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 13 | 0.31 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 13 | 0.31 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 13 | 0.31 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 19 | 0.31 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 3 | 0.31 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 3 | 0.31 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 3 | 0.31 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 8 | 0.31 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 15 | 0.31 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 6 | 0.31 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 15 | 0.31 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 12 | 0.31 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 15 | 0.31 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 14 | 0.31 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 16 | 0.31 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 16 | 0.31 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 16 | 0.31 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD21 | 8 | 0.31 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD22 | 8 | 0.31 |
| (1,57) | 1:47:A:LEU:HA | 1:47:A:LEU:HD23 | 8 | 0.31 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 13 | 0.31 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 13 | 0.31 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 13 | 0.31 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 8 | 0.3 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 8 | 0.3 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 8 | 0.3 |
| (1,924) | 1:62:A:ARG:HB3 | 1:63:A:GLN:HE21 | 6 | 0.3 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 6 | 0.3 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 6 | 0.3 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 6 | 0.3 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 6 | 0.3 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 6 | 0.3 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 6 | 0.3 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 2 | 0.3 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 2 | 0.3 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 2 | 0.3 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 10 | 0.3 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 13 | 0.3 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 4 | 0.3 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 4 | 0.3 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 4 | 0.3 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 17 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 17 | 0.3 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 17 | 0.3 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 5 | 0.3 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 7 | 0.3 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 7 | 0.3 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 7 | 0.3 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 1 | 0.3 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 1 | 0.3 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 1 | 0.3 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 18 | 0.3 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 18 | 0.3 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 18 | 0.3 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 5 | 0.3 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 5 | 0.3 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 5 | 0.3 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 15 | 0.3 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 15 | 0.3 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 15 | 0.3 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 17 | 0.29 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 17 | 0.29 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 17 | 0.29 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 19 | 0.29 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 19 | 0.29 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 19 | 0.29 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 19 | 0.29 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 19 | 0.29 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 19 | 0.29 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 16 | 0.29 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 16 | 0.29 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 16 | 0.29 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD11 | 10 | 0.29 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD12 | 10 | 0.29 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD13 | 10 | 0.29 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD11 | 4 | 0.29 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD12 | 4 | 0.29 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD13 | 4 | 0.29 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 18 | 0.29 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 14 | 0.29 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 14 | 0.29 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 14 | 0.29 |
| (1,370) | 1:50:A:ARG:HB2 | 1:51:A:ILE:H | 4 | 0.29 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 16 | 0.29 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 20 | 0.29 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 11 | 0.29 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 3 | 0.29 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG21 | 13 | 0.29 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG22 | 13 | 0.29 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG23 | 13 | 0.29 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 1 | 0.29 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 1 | 0.29 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 1 | 0.29 |
| (1,6) | 1:18:A:LEU:HD21 | 1:54:A:GLU:HG3 | 13 | 0.29 |
| (1,6) | 1:18:A:LEU:HD22 | 1:54:A:GLU:HG3 | 13 | 0.29 |
| (1,6) | 1:18:A:LEU:HD23 | 1:54:A:GLU:HG3 | 13 | 0.29 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 13 | 0.28 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 13 | 0.28 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD11 | 1:51:A:ILE:HD11 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD11 | 1:51:A:ILE:HD12 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD11 | 1:51:A:ILE:HD13 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD12 | 1:51:A:ILE:HD11 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD12 | 1:51:A:ILE:HD12 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD12 | 1:51:A:ILE:HD13 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD13 | 1:51:A:ILE:HD11 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD13 | 1:51:A:ILE:HD12 | 13 | 0.28 |
| (1,998) | 1:47:A:LEU:HD13 | 1:51:A:ILE:HD13 | 13 | 0.28 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 17 | 0.28 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 17 | 0.28 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 17 | 0.28 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 17 | 0.28 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 17 | 0.28 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 19 | 0.28 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 19 | 0.28 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 19 | 0.28 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 13 | 0.28 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 13 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 13 | 0.28 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 13 | 0.28 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 13 | 0.28 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 13 | 0.28 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 15 | 0.28 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 15 | 0.28 |
| (1,744) | 1:64:A:LEU:HB3 | 1:65:A:PHE:HB2 | 18 | 0.28 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 15 | 0.28 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 15 | 0.28 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 15 | 0.28 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 19 | 0.28 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 19 | 0.28 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 19 | 0.28 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 7 | 0.28 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 7 | 0.28 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 7 | 0.28 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 9 | 0.28 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 17 | 0.28 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 4 | 0.28 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 10 | 0.28 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 9 | 0.28 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 3 | 0.28 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 3 | 0.28 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 3 | 0.28 |
| (1,246) | 1:21:A:GLU:HG2 | 1:22:A:ILE:H | 8 | 0.28 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 17 | 0.28 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 17 | 0.28 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 17 | 0.28 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 6 | 0.28 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 6 | 0.28 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 6 | 0.28 |
| (1,40) | 1:25:A:VAL:HG11 | 1:37:A:LEU:HB2 | 19 | 0.28 |
| (1,40) | 1:25:A:VAL:HG12 | 1:37:A:LEU:HB2 | 19 | 0.28 |
| (1,40) | 1:25:A:VAL:HG13 | 1:37:A:LEU:HB2 | 19 | 0.28 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG11 | 3 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG12 | 3 | 0.28 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG13 | 3 | 0.28 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 19 | 0.27 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD21 | 12 | 0.27 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD22 | 12 | 0.27 |
| (1,1035) | 1:64:A:LEU:HA | 1:64:A:LEU:HD23 | 12 | 0.27 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 11 | 0.27 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 11 | 0.27 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 11 | 0.27 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 10 | 0.27 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 10 | 0.27 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 10 | 0.27 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 10 | 0.27 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 10 | 0.27 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 10 | 0.27 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 4 | 0.27 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 4 | 0.27 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD21 | 17 | 0.27 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD22 | 17 | 0.27 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD23 | 17 | 0.27 |
| (1,743) | 1:28:A:VAL:HG11 | 1:70:A:PRO:HB3 | 11 | 0.27 |
| (1,743) | 1:28:A:VAL:HG12 | 1:70:A:PRO:HB3 | 11 | 0.27 |
| (1,743) | 1:28:A:VAL:HG13 | 1:70:A:PRO:HB3 | 11 | 0.27 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD11 | 8 | 0.27 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD12 | 8 | 0.27 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD13 | 8 | 0.27 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD11 | 18 | 0.27 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD12 | 18 | 0.27 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD13 | 18 | 0.27 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 18 | 0.27 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 9 | 0.27 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 9 | 0.27 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 9 | 0.27 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 18 | 0.27 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 18 | 0.27 |
| (1,331) | 1:46:A:ARG:H | 1:46:A:ARG:HG3 | 18 | 0.27 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 3 | 0.27 |
| (1,269) | 1:26:A:GLU:HB2 | 1:27:A:ARG:H | 14 | 0.27 |
| (1,269) | 1:26:A:GLU:HB3 | 1:27:A:ARG:H | 14 | 0.27 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 9 | 0.27 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 9 | 0.27 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 9 | 0.27 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 20 | 0.27 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 20 | 0.27 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 20 | 0.27 |
| (1,125) | 1:27:A:ARG:HB2 | 1:27:A:ARG:HD2 | 2 | 0.27 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 20 | 0.27 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 20 | 0.27 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 20 | 0.27 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 4 | 0.27 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 4 | 0.27 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 4 | 0.27 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 5 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD11 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD12 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD11 | 1:64:A:LEU:HD13 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD11 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD12 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD12 | 1:64:A:LEU:HD13 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD11 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD12 | 12 | 0.26 |
| (1,1047) | 1:48:A:ILE:HD13 | 1:64:A:LEU:HD13 | 12 | 0.26 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 2 | 0.26 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 2 | 0.26 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 2 | 0.26 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 16 | 0.26 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 16 | 0.26 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD21 | 11 | 0.26 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD22 | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD23 | 11 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 6 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 6 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 6 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 11 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 11 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 11 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 17 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 17 | 0.26 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 17 | 0.26 |
| (1,751) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 12 | 0.26 |
| (1,751) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 12 | 0.26 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 9 | 0.26 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 9 | 0.26 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 9 | 0.26 |
| (1,699) | 1:23:A:LEU:HD21 | 1:37:A:LEU:H | 15 | 0.26 |
| (1,699) | 1:23:A:LEU:HD22 | 1:37:A:LEU:H | 15 | 0.26 |
| (1,699) | 1:23:A:LEU:HD23 | 1:37:A:LEU:H | 15 | 0.26 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 17 | 0.26 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 15 | 0.26 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 5 | 0.26 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 5 | 0.26 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 5 | 0.26 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 20 | 0.26 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 2 | 0.26 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 6 | 0.26 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 10 | 0.26 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 2 | 0.26 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 2 | 0.26 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 2 | 0.26 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 2 | 0.26 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 2 | 0.26 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 2 | 0.26 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 15 | 0.26 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 15 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 15 | 0.26 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 7 | 0.25 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 7 | 0.25 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 7 | 0.25 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD11 | 3 | 0.25 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD12 | 3 | 0.25 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD13 | 3 | 0.25 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG21 | 14 | 0.25 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG22 | 14 | 0.25 |
| (1,950) | 1:19:A:TYR:HE1 | 1:73:A:VAL:HG23 | 14 | 0.25 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG21 | 14 | 0.25 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG22 | 14 | 0.25 |
| (1,950) | 1:19:A:TYR:HE2 | 1:73:A:VAL:HG23 | 14 | 0.25 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 2 | 0.25 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 2 | 0.25 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 2 | 0.25 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 7 | 0.25 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 7 | 0.25 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 2 | 0.25 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 2 | 0.25 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 2 | 0.25 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 12 | 0.25 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 20 | 0.25 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 17 | 0.25 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 17 | 0.25 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 17 | 0.25 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 9 | 0.25 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 20 | 0.25 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 11 | 0.25 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 17 | 0.25 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 17 | 0.25 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 17 | 0.25 |
| (1,373) | 1:53:A:GLU:H | 1:53:A:GLU:HG3 | 20 | 0.25 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 6 | 0.25 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 10 | 0.25 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 11 | 0.25 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 11 | 0.25 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 11 | 0.25 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 10 | 0.25 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 10 | 0.25 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 10 | 0.25 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 19 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 19 | 0.25 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 19 | 0.25 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 16 | 0.25 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 16 | 0.25 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 16 | 0.25 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 14 | 0.25 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 9 | 0.24 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 9 | 0.24 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 9 | 0.24 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 9 | 0.24 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 9 | 0.24 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 9 | 0.24 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 20 | 0.24 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 20 | 0.24 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 20 | 0.24 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 4 | 0.24 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 4 | 0.24 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 11 | 0.24 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 11 | 0.24 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 11 | 0.24 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 9 | 0.24 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 9 | 0.24 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 9 | 0.24 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 3 | 0.24 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 15 | 0.24 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 15 | 0.24 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 15 | 0.24 |
| (1,443) | 1:62:A:ARG:HB3 | 1:64:A:LEU:H | 10 | 0.24 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 1 | 0.24 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 14 | 0.24 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 18 | 0.24 |
| (1,313) | 1:29:A:GLY:HA2 | 1:32:A:ASP:H | 18 | 0.24 |
| (1,267) | 1:20:A:ALA:HB1 | 1:28:A:VAL:H | 17 | 0.24 |
| (1,267) | 1:20:A:ALA:HB2 | 1:28:A:VAL:H | 17 | 0.24 |
| (1,267) | 1:20:A:ALA:HB3 | 1:28:A:VAL:H | 17 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG21 | 8 | 0.24 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG22 | 8 | 0.24 |
| (1,185) | 1:17:A:ALA:H | 1:28:A:VAL:HG23 | 8 | 0.24 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 10 | 0.24 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 10 | 0.24 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 10 | 0.24 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 17 | 0.23 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 14 | 0.23 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 6 | 0.23 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 6 | 0.23 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 6 | 0.23 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 6 | 0.23 |
| (1,767) | 1:75:A:ARG:HB2 | 1:75:A:ARG:HD2 | 15 | 0.23 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 20 | 0.23 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 20 | 0.23 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 20 | 0.23 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 4 | 0.23 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 17 | 0.23 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 16 | 0.23 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 16 | 0.23 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 16 | 0.23 |
| (1,362) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 2 | 0.23 |
| (1,316) | 1:23:A:LEU:HD11 | 1:39:A:GLY:H | 20 | 0.23 |
| (1,316) | 1:23:A:LEU:HD12 | 1:39:A:GLY:H | 20 | 0.23 |
| (1,316) | 1:23:A:LEU:HD13 | 1:39:A:GLY:H | 20 | 0.23 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 5 | 0.23 |
| (1,202) | 1:15:A:LEU:HB3 | 1:16:A:CYS:H | 3 | 0.23 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 15 | 0.23 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 15 | 0.23 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 15 | 0.23 |
| (1,92) | 1:26:A:GLU:HA | 1:26:A:GLU:HG2 | 16 | 0.23 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 1 | 0.22 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 9 | 0.22 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD11 | 8 | 0.22 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD12 | 8 | 0.22 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD13 | 8 | 0.22 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD11 | 8 | 0.22 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD12 | 8 | 0.22 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD13 | 8 | 0.22 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD11 | 8 | 0.22 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD12 | 8 | 0.22 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD13 | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 8 | 0.22 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 8 | 0.22 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 8 | 0.22 |
| (1,699) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD21 | 18 | 0.22 |
| (1,699) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD22 | 18 | 0.22 |
| (1,699) | 1:19:A:TYR:HD1 | 1:23:A:LEU:HD23 | 18 | 0.22 |
| (1,699) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD21 | 18 | 0.22 |
| (1,699) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD22 | 18 | 0.22 |
| (1,699) | 1:19:A:TYR:HD2 | 1:23:A:LEU:HD23 | 18 | 0.22 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 18 | 0.22 |
| (1,576) | 1:12:A:GLU:H | 1:13:A:LYS:HG3 | 1 | 0.22 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 1 | 0.22 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 1 | 0.22 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 1 | 0.22 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG21 | 6 | 0.22 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG22 | 6 | 0.22 |
| (1,471) | 1:69:A:THR:H | 1:73:A:VAL:HG23 | 6 | 0.22 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 17 | 0.22 |
| (1,408) | 1:57:A:VAL:HG21 | 1:59:A:LEU:H | 12 | 0.22 |
| (1,408) | 1:57:A:VAL:HG22 | 1:59:A:LEU:H | 12 | 0.22 |
| (1,408) | 1:57:A:VAL:HG23 | 1:59:A:LEU:H | 12 | 0.22 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 11 | 0.22 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 8 | 0.22 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 11 | 0.22 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 12 | 0.22 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 16 | 0.22 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 19 | 0.22 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 19 | 0.22 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 20 | 0.22 |
| (1,299) | 1:28:A:VAL:HG11 | 1:29:A:GLY:H | 18 | 0.22 |
| (1,299) | 1:28:A:VAL:HG12 | 1:29:A:GLY:H | 18 | 0.22 |
| (1,299) | 1:28:A:VAL:HG13 | 1:29:A:GLY:H | 18 | 0.22 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD21 | 10 | 0.22 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD22 | 10 | 0.22 |
| (1,295) | 1:32:A:ASP:H | 1:37:A:LEU:HD23 | 10 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 11 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 11 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 11 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 13 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 13 | 0.22 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 13 | 0.22 |
| (1,246) | 1:21:A:GLU:HG2 | 1:22:A:ILE:H | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,246) | 1:21:A:GLU:HG2 | 1:22:A:ILE:H | 10 | 0.22 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 4 | 0.22 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 4 | 0.22 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 13 | 0.21 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 6 | 0.21 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 6 | 0.21 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 6 | 0.21 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 14 | 0.21 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 14 | 0.21 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 9 | 0.21 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 9 | 0.21 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 9 | 0.21 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 13 | 0.21 |
| (1,840) | 1:11:A:THR:HG21 | 1:74:A:ALA:HA | 18 | 0.21 |
| (1,840) | 1:11:A:THR:HG22 | 1:74:A:ALA:HA | 18 | 0.21 |
| (1,840) | 1:11:A:THR:HG23 | 1:74:A:ALA:HA | 18 | 0.21 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG21 | 13 | 0.21 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG22 | 13 | 0.21 |
| (1,820) | 1:20:A:ALA:HA | 1:28:A:VAL:HG23 | 13 | 0.21 |
| (1,731) | 1:51:A:ILE:HG21 | 1:52:A:ARG:HG3 | 4 | 0.21 |
| (1,731) | 1:51:A:ILE:HG22 | 1:52:A:ARG:HG3 | 4 | 0.21 |
| (1,731) | 1:51:A:ILE:HG23 | 1:52:A:ARG:HG3 | 4 | 0.21 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 3 | 0.21 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 3 | 0.21 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 3 | 0.21 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 19 | 0.21 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 20 | 0.21 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB1 | 19 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB2 | 19 | 0.21 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB3 | 19 | 0.21 |
| (1,517) | 1:91:A:LYS:H | 1:91:A:LYS:HD3 | 16 | 0.21 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 2 | 0.21 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 16 | 0.21 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 3 | 0.21 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 7 | 0.21 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 12 | 0.21 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 12 | 0.21 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 12 | 0.21 |
| (1,125) | 1:27:A:ARG:HB2 | 1:27:A:ARG:HD2 | 8 | 0.21 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD11 | 5 | 0.21 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD12 | 5 | 0.21 |
| (1,113) | 1:61:A:ILE:HA | 1:64:A:LEU:HD13 | 5 | 0.21 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 8 | 0.21 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 8 | 0.21 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 8 | 0.21 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 16 | 0.21 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 1 | 0.21 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 1 | 0.21 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 10 | 0.2 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 15 | 0.2 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 8 | 0.2 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 14 | 0.2 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 14 | 0.2 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 14 | 0.2 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 17 | 0.2 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 17 | 0.2 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 17 | 0.2 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 15 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 15 | 0.2 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 15 | 0.2 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 1 | 0.2 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 15 | 0.2 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 15 | 0.2 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 15 | 0.2 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 15 | 0.2 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 15 | 0.2 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 15 | 0.2 |
| (1,924) | 1:62:A:ARG:HB3 | 1:63:A:GLN:HE21 | 9 | 0.2 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 19 | 0.2 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD21 | 4 | 0.2 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD22 | 4 | 0.2 |
| (1,804) | 1:48:A:ILE:HG12 | 1:59:A:LEU:HD23 | 4 | 0.2 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 2 | 0.2 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 2 | 0.2 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 4 | 0.2 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 4 | 0.2 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 4 | 0.2 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 14 | 0.2 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 14 | 0.2 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 14 | 0.2 |
| (1,684) | 1:64:A:LEU:HD21 | 1:68:A:PRO:HA | 12 | 0.2 |
| (1,684) | 1:64:A:LEU:HD22 | 1:68:A:PRO:HA | 12 | 0.2 |
| (1,684) | 1:64:A:LEU:HD23 | 1:68:A:PRO:HA | 12 | 0.2 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 4 | 0.2 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 4 | 0.2 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 4 | 0.2 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 16 | 0.2 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 2 | 0.2 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 6 | 0.2 |
| (1,495) | 1:75:A:ARG:H | 1:75:A:ARG:HG3 | 5 | 0.2 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 9 | 0.2 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 2 | 0.2 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 2 | 0.2 |
| (1,408) | 1:57:A:VAL:HG21 | 1:59:A:LEU:H | 5 | 0.2 |
| (1,408) | 1:57:A:VAL:HG22 | 1:59:A:LEU:H | 5 | 0.2 |
| (1,408) | 1:57:A:VAL:HG23 | 1:59:A:LEU:H | 5 | 0.2 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 2 | 0.2 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 14 | 0.2 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 7 | 0.2 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 4 | 0.2 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 4 | 0.2 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 4 | 0.2 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 3 | 0.2 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 3 | 0.2 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 3 | 0.2 |
| (1,86) | 1:52:A:ARG:HA | 1:52:A:ARG:HD2 | 19 | 0.2 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG11 | 10 | 0.2 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG12 | 10 | 0.2 |
| (1,75) | 1:63:A:GLN:HB2 | 1:73:A:VAL:HG13 | 10 | 0.2 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 9 | 0.2 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 9 | 0.2 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 9 | 0.2 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 18 | 0.2 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 18 | 0.2 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 18 | 0.2 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 16 | 0.19 |
| (1,1034) | 1:42:A:ALA:HA | 1:45:A:MET:HG2 | 20 | 0.19 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 18 | 0.19 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 3 | 0.19 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 3 | 0.19 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 3 | 0.19 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 3 | 0.19 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 3 | 0.19 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 3 | 0.19 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 18 | 0.19 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 18 | 0.19 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 18 | 0.19 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 10 | 0.19 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 10 | 0.19 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 10 | 0.19 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 1 | 0.19 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 18 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 18 | 0.19 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 18 | 0.19 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG11 | 10 | 0.19 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG12 | 10 | 0.19 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG13 | 10 | 0.19 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 19 | 0.19 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 19 | 0.19 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 5 | 0.19 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 5 | 0.19 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 5 | 0.19 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 9 | 0.19 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 9 | 0.19 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 9 | 0.19 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD11 | 2 | 0.19 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD12 | 2 | 0.19 |
| (1,637) | 1:15:A:LEU:H | 1:18:A:LEU:HD13 | 2 | 0.19 |
| (1,576) | 1:12:A:GLU:H | 1:13:A:LYS:HG3 | 16 | 0.19 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 13 | 0.19 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 13 | 0.19 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 13 | 0.19 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 19 | 0.19 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 1 | 0.19 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 14 | 0.19 |
| (1,362) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 16 | 0.19 |
| (1,333) | 1:45:A:MET:H | 1:45:A:MET:HB3 | 13 | 0.19 |
| (1,316) | 1:23:A:LEU:HD11 | 1:39:A:GLY:H | 4 | 0.19 |
| (1,316) | 1:23:A:LEU:HD12 | 1:39:A:GLY:H | 4 | 0.19 |
| (1,316) | 1:23:A:LEU:HD13 | 1:39:A:GLY:H | 4 | 0.19 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 3 | 0.19 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 18 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,270) | 1:26:A:GLU:HG2 | 1:27:A:ARG:H | 16 | 0.19 |
| (1,202) | 1:15:A:LEU:HB3 | 1:16:A:CYS:H | 7 | 0.19 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 20 | 0.19 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 20 | 0.19 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 20 | 0.19 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 8 | 0.19 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 8 | 0.19 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD21 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD22 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD11 | 1:64:A:LEU:HD23 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD21 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD22 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD12 | 1:64:A:LEU:HD23 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD21 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD22 | 8 | 0.19 |
| (1,61) | 1:47:A:LEU:HD13 | 1:64:A:LEU:HD23 | 8 | 0.19 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 15 | 0.19 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 15 | 0.19 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 15 | 0.19 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 6 | 0.19 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 6 | 0.19 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 6 | 0.19 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 13 | 0.18 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 13 | 0.18 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 13 | 0.18 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 5 | 0.18 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 5 | 0.18 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 5 | 0.18 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 4 | 0.18 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 4 | 0.18 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 5 | 0.18 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 5 | 0.18 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 5 | 0.18 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 10 | 0.18 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 10 | 0.18 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 12 | 0.18 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 12 | 0.18 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 4 | 0.18 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 4 | 0.18 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 4 | 0.18 |
| (1,869) | 1:46:A:ARG:HA | 1:46:A:ARG:HD2 | 4 | 0.18 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 17 | 0.18 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 13 | 0.18 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 13 | 0.18 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 10 | 0.18 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 10 | 0.18 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 3 | 0.18 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 3 | 0.18 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 3 | 0.18 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD11 | 9 | 0.18 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD12 | 9 | 0.18 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD13 | 9 | 0.18 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 12 | 0.18 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 12 | 0.18 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 12 | 0.18 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG21 | 15 | 0.18 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG22 | 15 | 0.18 |
| (1,505) | 1:73:A:VAL:H | 1:73:A:VAL:HG23 | 15 | 0.18 |
| (1,494) | 1:75:A:ARG:H | 1:75:A:ARG:HB3 | 8 | 0.18 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 17 | 0.18 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 17 | 0.18 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD11 | 7 | 0.18 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD12 | 7 | 0.18 |
| (1,477) | 1:76:A:ALA:H | 1:77:A:LEU:HD13 | 7 | 0.18 |
| (1,443) | 1:62:A:ARG:HB3 | 1:64:A:LEU:H | 14 | 0.18 |
| (1,436) | 1:64:A:LEU:HD11 | 1:65:A:PHE:H | 12 | 0.18 |
| (1,436) | 1:64:A:LEU:HD12 | 1:65:A:PHE:H | 12 | 0.18 |
| (1,436) | 1:64:A:LEU:HD13 | 1:65:A:PHE:H | 12 | 0.18 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 8 | 0.18 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 12 | 0.18 |
| (1,350) | 1:47:A:LEU:HD11 | 1:48:A:ILE:H | 13 | 0.18 |
| (1,350) | 1:47:A:LEU:HD12 | 1:48:A:ILE:H | 13 | 0.18 |
| (1,350) | 1:47:A:LEU:HD13 | 1:48:A:ILE:H | 13 | 0.18 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 2 | 0.18 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 5 | 0.18 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 7 | 0.18 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 7 | 0.18 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 10 | 0.18 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 10 | 0.18 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 10 | 0.18 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 4 | 0.17 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 10 | 0.17 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 4 | 0.17 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 4 | 0.17 |
| (1,1019) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 4 | 0.17 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 2 | 0.17 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 2 | 0.17 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 14 | 0.17 |
| (1,854) | 1:27:A:ARG:HB2 | 1:28:A:VAL:HA | 8 | 0.17 |
| (1,811) | 1:63:A:GLN:HA | 1:77:A:LEU:HB3 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG21 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG22 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG23 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG21 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG22 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG23 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG21 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG22 | 20 | 0.17 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG23 | 20 | 0.17 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD21 | 15 | 0.17 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD22 | 15 | 0.17 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD23 | 15 | 0.17 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 3 | 0.17 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 3 | 0.17 |
| (1,735) | 1:18:A:LEU:HD11 | 1:51:A:ILE:HA | 17 | 0.17 |
| (1,735) | 1:18:A:LEU:HD12 | 1:51:A:ILE:HA | 17 | 0.17 |
| (1,735) | 1:18:A:LEU:HD13 | 1:51:A:ILE:HA | 17 | 0.17 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 2 | 0.17 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 2 | 0.17 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 2 | 0.17 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 11 | 0.17 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 11 | 0.17 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 11 | 0.17 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 14 | 0.17 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 14 | 0.17 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 14 | 0.17 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD11 | 12 | 0.17 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD12 | 12 | 0.17 |
| (1,667) | 1:34:A:PHE:HZ | 1:47:A:LEU:HD13 | 12 | 0.17 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB1 | 20 | 0.17 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB2 | 20 | 0.17 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB3 | 20 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,443) | 1:62:A:ARG:HB3 | 1:64:A:LEU:H | 17 | 0.17 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 16 | 0.17 |
| (1,396) | 1:18:A:LEU:HD11 | 1:54:A:GLU:H | 4 | 0.17 |
| (1,396) | 1:18:A:LEU:HD12 | 1:54:A:GLU:H | 4 | 0.17 |
| (1,396) | 1:18:A:LEU:HD13 | 1:54:A:GLU:H | 4 | 0.17 |
| (1,369) | 1:50:A:ARG:H | 1:50:A:ARG:HB3 | 13 | 0.17 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 17 | 0.17 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 17 | 0.17 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 17 | 0.17 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 17 | 0.17 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD21 | 9 | 0.17 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD22 | 9 | 0.17 |
| (1,185) | 1:17:A:ALA:H | 1:18:A:LEU:HD23 | 9 | 0.17 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 1 | 0.17 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 1 | 0.17 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 1 | 0.17 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 3 | 0.17 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 3 | 0.17 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 3 | 0.17 |
| (1,40) | 1:25:A:VAL:HG11 | 1:37:A:LEU:HB2 | 15 | 0.17 |
| (1,40) | 1:25:A:VAL:HG12 | 1:37:A:LEU:HB2 | 15 | 0.17 |
| (1,40) | 1:25:A:VAL:HG13 | 1:37:A:LEU:HB2 | 15 | 0.17 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 8 | 0.17 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 8 | 0.17 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 8 | 0.17 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 12 | 0.16 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD11 | 4 | 0.16 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD12 | 4 | 0.16 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD13 | 4 | 0.16 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 3 | 0.16 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 3 | 0.16 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 3 | 0.16 |
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 15 | 0.16 |
| (1,924) | 1:62:A:ARG:HB3 | 1:63:A:GLN:HE21 | 14 | 0.16 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 5 | 0.16 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 5 | 0.16 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 5 | 0.16 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG11 | 8 | 0.16 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG12 | 8 | 0.16 |
| (1,799) | 1:11:A:THR:HA | 1:14:A:VAL:HG13 | 8 | 0.16 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 9 | 0.16 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 9 | 0.16 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 14 | 0.16 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 14 | 0.16 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 1 | 0.16 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 1 | 0.16 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 1 | 0.16 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 18 | 0.16 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 18 | 0.16 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 18 | 0.16 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 10 | 0.16 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 10 | 0.16 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 10 | 0.16 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 12 | 0.16 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 18 | 0.16 |
| (1,418) | 1:54:A:GLU:HG3 | 1:55:A:LEU:H | 14 | 0.16 |
| (1,373) | 1:53:A:GLU:H | 1:53:A:GLU:HG3 | 4 | 0.16 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 6 | 0.16 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 8 | 0.16 |
| (1,249) | 1:22:A:ILE:H | 1:22:A:ILE:HG13 | 16 | 0.16 |
| (1,209) | 1:21:A:GLU:HB2 | 1:22:A:ILE:H | 18 | 0.16 |
| (1,209) | 1:21:A:GLU:HB3 | 1:22:A:ILE:H | 18 | 0.16 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 19 | 0.16 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 19 | 0.16 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 19 | 0.16 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 20 | 0.16 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 20 | 0.16 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 20 | 0.16 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 15 | 0.16 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 15 | 0.16 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 15 | 0.16 |
| (1,40) | 1:25:A:VAL:HG11 | 1:37:A:LEU:HB2 | 6 | 0.16 |
| (1,40) | 1:25:A:VAL:HG12 | 1:37:A:LEU:HB2 | 6 | 0.16 |
| (1,40) | 1:25:A:VAL:HG13 | 1:37:A:LEU:HB2 | 6 | 0.16 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 17 | 0.16 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 17 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 17 | 0.16 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG21 | 11 | 0.16 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG22 | 11 | 0.16 |
| (1,22) | 1:16:A:CYS:HB3 | 1:28:A:VAL:HG23 | 11 | 0.16 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 18 | 0.16 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 18 | 0.16 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 18 | 0.16 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 8 | 0.15 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 2 | 0.15 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 2 | 0.15 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 2 | 0.15 |
| (1,985) | 1:47:A:LEU:H | 1:48:A:ILE:HD11 | 18 | 0.15 |
| (1,985) | 1:47:A:LEU:H | 1:48:A:ILE:HD12 | 18 | 0.15 |
| (1,985) | 1:47:A:LEU:H | 1:48:A:ILE:HD13 | 18 | 0.15 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 11 | 0.15 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 11 | 0.15 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 11 | 0.15 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE1 | 5 | 0.15 |
| (1,814) | 1:64:A:LEU:HD11 | 1:65:A:PHE:HE2 | 5 | 0.15 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE1 | 5 | 0.15 |
| (1,814) | 1:64:A:LEU:HD12 | 1:65:A:PHE:HE2 | 5 | 0.15 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE1 | 5 | 0.15 |
| (1,814) | 1:64:A:LEU:HD13 | 1:65:A:PHE:HE2 | 5 | 0.15 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 3 | 0.15 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 3 | 0.15 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 3 | 0.15 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 10 | 0.15 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 10 | 0.15 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 10 | 0.15 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 19 | 0.15 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 19 | 0.15 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 19 | 0.15 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 19 | 0.15 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 19 | 0.15 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 19 | 0.15 |
| (1,622) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 2 | 0.15 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 12 | 0.15 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 14 | 0.15 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 19 | 0.15 |
| (1,370) | 1:50:A:ARG:HB2 | 1:51:A:ILE:H | 9 | 0.15 |
| (1,370) | 1:50:A:ARG:HB2 | 1:51:A:ILE:H | 11 | 0.15 |
| (1,364) | 1:52:A:ARG:HD2 | 1:53:A:GLU:H | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 4 | 0.15 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG21 | 18 | 0.15 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG22 | 18 | 0.15 |
| (1,220) | 1:19:A:TYR:H | 1:28:A:VAL:HG23 | 18 | 0.15 |
| (1,209) | 1:21:A:GLU:HB2 | 1:22:A:ILE:H | 6 | 0.15 |
| (1,209) | 1:21:A:GLU:HB3 | 1:22:A:ILE:H | 6 | 0.15 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 9 | 0.15 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 9 | 0.15 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 9 | 0.15 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 2 | 0.15 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 2 | 0.15 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 2 | 0.15 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 14 | 0.15 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 14 | 0.15 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 14 | 0.15 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 3 | 0.15 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 3 | 0.15 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 3 | 0.15 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 7 | 0.15 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 7 | 0.15 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 7 | 0.15 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG11 | 19 | 0.15 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG12 | 19 | 0.15 |
| (1,27) | 1:12:A:GLU:HB2 | 1:30:A:VAL:HG13 | 19 | 0.15 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 16 | 0.15 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 16 | 0.15 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 16 | 0.15 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 7 | 0.14 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 15 | 0.14 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD11 | 7 | 0.14 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD12 | 7 | 0.14 |
| (1,1003) | 1:14:A:VAL:H | 1:15:A:LEU:HD13 | 7 | 0.14 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 9 | 0.14 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 9 | 0.14 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 12 | 0.14 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 17 | 0.14 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 8 | 0.14 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 8 | 0.14 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 8 | 0.14 |
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 8 | 0.14 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 16 | 0.14 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 16 | 0.14 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 1 | 0.14 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 1 | 0.14 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 1 | 0.14 |
| (1,866) | 1:54:A:GLU:HA | 1:54:A:GLU:HG2 | 13 | 0.14 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 15 | 0.14 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 15 | 0.14 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 15 | 0.14 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 15 | 0.14 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 15 | 0.14 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 15 | 0.14 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 9 | 0.14 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 9 | 0.14 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 9 | 0.14 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 2 | 0.14 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 7 | 0.14 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 8 | 0.14 |
| (1,519) | 1:27:A:ARG:H | 1:27:A:ARG:HB3 | 18 | 0.14 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB1 | 4 | 0.14 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB2 | 4 | 0.14 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB3 | 4 | 0.14 |
| (1,443) | 1:62:A:ARG:HB3 | 1:64:A:LEU:H | 11 | 0.14 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 2 | 0.14 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 4 | 0.14 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 6 | 0.14 |
| (1,373) | 1:53:A:GLU:H | 1:53:A:GLU:HG3 | 12 | 0.14 |
| (1,362) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 8 | 0.14 |
| (1,303) | 1:31:A:ASP:H | 1:31:A:ASP:HB3 | 13 | 0.14 |
| (1,249) | 1:22:A:ILE:H | 1:22:A:ILE:HG13 | 4 | 0.14 |
| (1,216) | 1:15:A:LEU:HA | 1:17:A:ALA:H | 20 | 0.14 |
| (1,209) | 1:21:A:GLU:HB2 | 1:22:A:ILE:H | 16 | 0.14 |
| (1,209) | 1:21:A:GLU:HB3 | 1:22:A:ILE:H | 16 | 0.14 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 4 | 0.14 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 4 | 0.14 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 6 | 0.14 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 6 | 0.14 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 6 | 0.14 |
| (1,78) | 1:50:A:ARG:HB2 | 1:51:A:ILE:HA | 8 | 0.14 |
| (1,40) | 1:25:A:VAL:HG11 | 1:37:A:LEU:HB2 | 9 | 0.14 |
| (1,40) | 1:25:A:VAL:HG12 | 1:37:A:LEU:HB2 | 9 | 0.14 |
| (1,40) | 1:25:A:VAL:HG13 | 1:37:A:LEU:HB2 | 9 | 0.14 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 11 | 0.14 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 11 | 0.14 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 11 | 0.14 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 9 | 0.13 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 3 | 0.13 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 3 | 0.13 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 3 | 0.13 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 15 | 0.13 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 15 | 0.13 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 15 | 0.13 |
| (1,986) | 1:66:A:SER:HB2 | 1:67:A:SER:H | 5 | 0.13 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD11 | 4 | 0.13 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD12 | 4 | 0.13 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD13 | 4 | 0.13 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD11 | 4 | 0.13 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD12 | 4 | 0.13 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD13 | 4 | 0.13 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 19 | 0.13 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 19 | 0.13 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 19 | 0.13 |
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 13 | 0.13 |
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 19 | 0.13 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 14 | 0.13 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 14 | 0.13 |
| (1,923) | 1:63:A:GLN:HB2 | 1:63:A:GLN:HE21 | 18 | 0.13 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 7 | 0.13 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 7 | 0.13 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 7 | 0.13 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 12 | 0.13 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 12 | 0.13 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 12 | 0.13 |
| (1,888) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 18 | 0.13 |
| (1,888) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 18 | 0.13 |
| (1,888) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 18 | 0.13 |
| (1,842) | 1:20:A:ALA:HB1 | 1:27:A:ARG:HA | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,842) | 1:20:A:ALA:HB2 | 1:27:A:ARG:HA | 14 | 0.13 |
| (1,842) | 1:20:A:ALA:HB3 | 1:27:A:ARG:HA | 14 | 0.13 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 11 | 0.13 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 11 | 0.13 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG21 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG22 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG21 | 1:14:A:VAL:HG23 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG21 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG22 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG22 | 1:14:A:VAL:HG23 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG21 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG22 | 18 | 0.13 |
| (1,802) | 1:11:A:THR:HG23 | 1:14:A:VAL:HG23 | 18 | 0.13 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 2 | 0.13 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 2 | 0.13 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD21 | 9 | 0.13 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD22 | 9 | 0.13 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD23 | 9 | 0.13 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG21 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG22 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG23 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG21 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG22 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG23 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG21 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG22 | 15 | 0.13 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG23 | 15 | 0.13 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD21 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD22 | 17 | 0.13 |
| (1,723) | 1:22:A:ILE:HB | 1:47:A:LEU:HD23 | 17 | 0.13 |
| (1,700) | 1:34:A:PHE:HD1 | 1:47:A:LEU:HD11 | 8 | 0.13 |
| (1,700) | 1:34:A:PHE:HD1 | 1:47:A:LEU:HD12 | 8 | 0.13 |
| (1,700) | 1:34:A:PHE:HD1 | 1:47:A:LEU:HD13 | 8 | 0.13 |
| (1,700) | 1:34:A:PHE:HD2 | 1:47:A:LEU:HD11 | 8 | 0.13 |
| (1,700) | 1:34:A:PHE:HD2 | 1:47:A:LEU:HD12 | 8 | 0.13 |
| (1,700) | 1:34:A:PHE:HD2 | 1:47:A:LEU:HD13 | 8 | 0.13 |
| (1,699) | 1:23:A:LEU:HD21 | 1:37:A:LEU:H | 5 | 0.13 |
| (1,699) | 1:23:A:LEU:HD22 | 1:37:A:LEU:H | 5 | 0.13 |
| (1,699) | 1:23:A:LEU:HD23 | 1:37:A:LEU:H | 5 | 0.13 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 6 | 0.13 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 14 | 0.13 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 5 | 0.13 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 9 | 0.13 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 11 | 0.13 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 13 | 0.13 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 16 | 0.13 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB1 | 6 | 0.13 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB2 | 6 | 0.13 |
| (1,589) | 1:32:A:ASP:H | 1:71:A:ALA:HB3 | 6 | 0.13 |
| (1,588) | 1:30:A:VAL:H | 1:31:A:ASP:HB3 | 13 | 0.13 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 17 | 0.13 |
| (1,418) | 1:54:A:GLU:HG3 | 1:55:A:LEU:H | 8 | 0.13 |
| (1,350) | 1:47:A:LEU:HD11 | 1:48:A:ILE:H | 18 | 0.13 |
| (1,350) | 1:47:A:LEU:HD12 | 1:48:A:ILE:H | 18 | 0.13 |
| (1,350) | 1:47:A:LEU:HD13 | 1:48:A:ILE:H | 18 | 0.13 |
| (1,316) | 1:23:A:LEU:HD11 | 1:39:A:GLY:H | 13 | 0.13 |
| (1,316) | 1:23:A:LEU:HD12 | 1:39:A:GLY:H | 13 | 0.13 |
| (1,316) | 1:23:A:LEU:HD13 | 1:39:A:GLY:H | 13 | 0.13 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 18 | 0.13 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 18 | 0.13 |
| (1,274) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 18 | 0.13 |
| (1,269) | 1:26:A:GLU:HB2 | 1:27:A:ARG:H | 17 | 0.13 |
| (1,269) | 1:26:A:GLU:HB3 | 1:27:A:ARG:H | 17 | 0.13 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD21 | 3 | 0.13 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD22 | 3 | 0.13 |
| (1,186) | 1:18:A:LEU:H | 1:18:A:LEU:HD23 | 3 | 0.13 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 7 | 0.13 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 7 | 0.13 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 7 | 0.13 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 18 | 0.13 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 18 | 0.13 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 5 | 0.13 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 5 | 0.13 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 5 | 0.13 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 15 | 0.13 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 15 | 0.13 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 15 | 0.13 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD11 | 7 | 0.13 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD12 | 7 | 0.13 |
| (1,181) | 1:15:A:LEU:H | 1:15:A:LEU:HD13 | 7 | 0.13 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 12 | 0.13 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 12 | 0.13 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 12 | 0.13 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 14 | 0.13 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 14 | 0.13 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 14 | 0.13 |
| (1,1050) | 1:53:A:GLU:HA | 1:53:A:GLU:HG3 | 3 | 0.12 |
| (1,1028) | 1:51:A:ILE:HA | 1:54:A:GLU:HB3 | 19 | 0.12 |
| (1,1007) | 1:27:A:ARG:HA | 1:27:A:ARG:HD2 | 10 | 0.12 |
| (1,1007) | 1:27:A:ARG:HA | 1:27:A:ARG:HD3 | 10 | 0.12 |
| (1,955) | 1:11:A:THR:HA | 1:14:A:VAL:H | 5 | 0.12 |
| (1,934) | 1:23:A:LEU:HD11 | 1:34:A:PHE:HZ | 7 | 0.12 |
| (1,934) | 1:23:A:LEU:HD12 | 1:34:A:PHE:HZ | 7 | 0.12 |
| (1,934) | 1:23:A:LEU:HD13 | 1:34:A:PHE:HZ | 7 | 0.12 |
| (1,924) | 1:62:A:ARG:HB3 | 1:63:A:GLN:HE21 | 16 | 0.12 |
| (1,919) | 1:45:A:MET:H | 1:48:A:ILE:HD11 | 19 | 0.12 |
| (1,919) | 1:45:A:MET:H | 1:48:A:ILE:HD12 | 19 | 0.12 |
| (1,919) | 1:45:A:MET:H | 1:48:A:ILE:HD13 | 19 | 0.12 |
| (1,891) | 1:69:A:THR:HG21 | 1:71:A:ALA:H | 9 | 0.12 |
| (1,891) | 1:69:A:THR:HG22 | 1:71:A:ALA:H | 9 | 0.12 |
| (1,891) | 1:69:A:THR:HG23 | 1:71:A:ALA:H | 9 | 0.12 |
| (1,869) | 1:46:A:ARG:HA | 1:46:A:ARG:HD2 | 14 | 0.12 |
| (1,811) | 1:63:A:GLN:HA | 1:77:A:LEU:HB3 | 12 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 17 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 17 | 0.12 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 17 | 0.12 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD21 | 13 | 0.12 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD22 | 13 | 0.12 |
| (1,785) | 1:19:A:TYR:HA | 1:47:A:LEU:HD23 | 13 | 0.12 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB1 | 16 | 0.12 |
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB2 | 16 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,758) | 1:40:A:SER:HB2 | 1:42:A:ALA:HB3 | 16 | 0.12 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD21 | 8 | 0.12 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD22 | 8 | 0.12 |
| (1,753) | 1:32:A:ASP:HB2 | 1:37:A:LEU:HD23 | 8 | 0.12 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG11 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG12 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD21 | 1:73:A:VAL:HG13 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG11 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG12 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD22 | 1:73:A:VAL:HG13 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG11 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG12 | 18 | 0.12 |
| (1,748) | 1:64:A:LEU:HD23 | 1:73:A:VAL:HG13 | 18 | 0.12 |
| (1,742) | 1:28:A:VAL:HG11 | 1:32:A:ASP:HB2 | 12 | 0.12 |
| (1,742) | 1:28:A:VAL:HG12 | 1:32:A:ASP:HB2 | 12 | 0.12 |
| (1,742) | 1:28:A:VAL:HG13 | 1:32:A:ASP:HB2 | 12 | 0.12 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 7 | 0.12 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 7 | 0.12 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 7 | 0.12 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG21 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG22 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG23 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG21 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG22 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG23 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG21 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG22 | 19 | 0.12 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG23 | 19 | 0.12 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD11 | 5 | 0.12 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD12 | 5 | 0.12 |
| (1,726) | 1:12:A:GLU:HG3 | 1:15:A:LEU:HD13 | 5 | 0.12 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD1 | 16 | 0.12 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD2 | 16 | 0.12 |
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD1 | 16 | 0.12 |
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD2 | 16 | 0.12 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD1 | 16 | 0.12 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD2 | 16 | 0.12 |
| (1,699) | 1:23:A:LEU:HD21 | 1:37:A:LEU:H | 4 | 0.12 |
| (1,699) | 1:23:A:LEU:HD22 | 1:37:A:LEU:H | 4 | 0.12 |
| (1,699) | 1:23:A:LEU:HD23 | 1:37:A:LEU:H | 4 | 0.12 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG11 | 11 | 0.12 |
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG12 | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,607) | 1:69:A:THR:H | 1:73:A:VAL:HG13 | 11 | 0.12 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 14 | 0.12 |
| (1,590) | 1:32:A:ASP:H | 1:70:A:PRO:HB3 | 19 | 0.12 |
| (1,519) | 1:27:A:ARG:H | 1:27:A:ARG:HB3 | 5 | 0.12 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 5 | 0.12 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 5 | 0.12 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 5 | 0.12 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB1 | 16 | 0.12 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB2 | 16 | 0.12 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB3 | 16 | 0.12 |
| (1,418) | 1:54:A:GLU:HG3 | 1:55:A:LEU:H | 15 | 0.12 |
| (1,412) | 1:55:A:LEU:HG | 1:56:A:GLY:H | 19 | 0.12 |
| (1,377) | 1:54:A:GLU:H | 1:54:A:GLU:HB3 | 16 | 0.12 |
| (1,267) | 1:20:A:ALA:HB1 | 1:28:A:VAL:H | 1 | 0.12 |
| (1,267) | 1:20:A:ALA:HB2 | 1:28:A:VAL:H | 1 | 0.12 |
| (1,267) | 1:20:A:ALA:HB3 | 1:28:A:VAL:H | 1 | 0.12 |
| (1,259) | 1:23:A:LEU:H | 1:23:A:LEU:HD21 | 9 | 0.12 |
| (1,259) | 1:23:A:LEU:H | 1:23:A:LEU:HD22 | 9 | 0.12 |
| (1,259) | 1:23:A:LEU:H | 1:23:A:LEU:HD23 | 9 | 0.12 |
| (1,249) | 1:22:A:ILE:H | 1:22:A:ILE:HG13 | 14 | 0.12 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 11 | 0.12 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 11 | 0.12 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 11 | 0.12 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 13 | 0.12 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 13 | 0.12 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 13 | 0.12 |
| (1,183) | 1:15:A:LEU:HD11 | 1:16:A:CYS:H | 17 | 0.12 |
| (1,183) | 1:15:A:LEU:HD12 | 1:16:A:CYS:H | 17 | 0.12 |
| (1,183) | 1:15:A:LEU:HD13 | 1:16:A:CYS:H | 17 | 0.12 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 17 | 0.12 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 17 | 0.12 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 17 | 0.12 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 1 | 0.12 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 1 | 0.12 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 1 | 0.12 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 2 | 0.12 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 2 | 0.12 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 2 | 0.12 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 17 | 0.12 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 17 | 0.12 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 17 | 0.12 |
| (1,1034) | 1:42:A:ALA:HA | 1:45:A:MET:HG2 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 1 | 0.11 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 1 | 0.11 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 1 | 0.11 |
| (1,1026) | 1:51:A:ILE:HD11 | 1:60:A:PRO:HD2 | 5 | 0.11 |
| (1,1026) | 1:51:A:ILE:HD12 | 1:60:A:PRO:HD2 | 5 | 0.11 |
| (1,1026) | 1:51:A:ILE:HD13 | 1:60:A:PRO:HD2 | 5 | 0.11 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD11 | 10 | 0.11 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD12 | 10 | 0.11 |
| (1,1016) | 1:14:A:VAL:HB | 1:55:A:LEU:HD13 | 10 | 0.11 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD11 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD12 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG21 | 1:23:A:LEU:HD13 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD11 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD12 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG22 | 1:23:A:LEU:HD13 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD11 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD12 | 1 | 0.11 |
| (1,994) | 1:22:A:ILE:HG23 | 1:23:A:LEU:HD13 | 1 | 0.11 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD11 | 16 | 0.11 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD12 | 16 | 0.11 |
| (1,939) | 1:34:A:PHE:HE1 | 1:43:A:LEU:HD13 | 16 | 0.11 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD11 | 16 | 0.11 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD12 | 16 | 0.11 |
| (1,939) | 1:34:A:PHE:HE2 | 1:43:A:LEU:HD13 | 16 | 0.11 |
| (1,925) | 1:62:A:ARG:HG2 | 1:63:A:GLN:HE21 | 10 | 0.11 |
| (1,925) | 1:62:A:ARG:HG3 | 1:63:A:GLN:HE21 | 10 | 0.11 |
| (1,868) | 1:27:A:ARG:HA | 1:27:A:ARG:HG3 | 2 | 0.11 |
| (1,853) | 1:91:A:LYS:HA | 1:91:A:LYS:HD3 | 13 | 0.11 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 14 | 0.11 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 14 | 0.11 |
| (1,811) | 1:63:A:GLN:HA | 1:77:A:LEU:HB3 | 10 | 0.11 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 13 | 0.11 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 13 | 0.11 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 13 | 0.11 |
| (1,784) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 16 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,784) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 18 | 0.11 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 2 | 0.11 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 2 | 0.11 |
| (1,769) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 2 | 0.11 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 3 | 0.11 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 3 | 0.11 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG21 | 15 | 0.11 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG22 | 15 | 0.11 |
| (1,733) | 1:17:A:ALA:HA | 1:28:A:VAL:HG23 | 15 | 0.11 |
| (1,730) | 1:51:A:ILE:HG21 | 1:59:A:LEU:HB3 | 8 | 0.11 |
| (1,730) | 1:51:A:ILE:HG22 | 1:59:A:LEU:HB3 | 8 | 0.11 |
| (1,730) | 1:51:A:ILE:HG23 | 1:59:A:LEU:HB3 | 8 | 0.11 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG21 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG22 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG21 | 1:51:A:ILE:HG23 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG21 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG22 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG22 | 1:51:A:ILE:HG23 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG21 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG22 | 3 | 0.11 |
| (1,729) | 1:48:A:ILE:HG23 | 1:51:A:ILE:HG23 | 3 | 0.11 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 1 | 0.11 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 1 | 0.11 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 1 | 0.11 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 1 | 0.11 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 1 | 0.11 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 1 | 0.11 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG2 | 13 | 0.11 |
| (1,721) | 1:59:A:LEU:HD21 | 1:63:A:GLN:HG3 | 13 | 0.11 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG2 | 13 | 0.11 |
| (1,721) | 1:59:A:LEU:HD22 | 1:63:A:GLN:HG3 | 13 | 0.11 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG2 | 13 | 0.11 |
| (1,721) | 1:59:A:LEU:HD23 | 1:63:A:GLN:HG3 | 13 | 0.11 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD1 | 5 | 0.11 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD2 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD1 | 5 | 0.11 |
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD2 | 5 | 0.11 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD1 | 5 | 0.11 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD2 | 5 | 0.11 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD1 | 17 | 0.11 |
| (1,709) | 1:44:A:ALA:HB1 | 1:65:A:PHE:HD2 | 17 | 0.11 |
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD1 | 17 | 0.11 |
| (1,709) | 1:44:A:ALA:HB2 | 1:65:A:PHE:HD2 | 17 | 0.11 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD1 | 17 | 0.11 |
| (1,709) | 1:44:A:ALA:HB3 | 1:65:A:PHE:HD2 | 17 | 0.11 |
| (1,593) | 1:45:A:MET:HB3 | 1:47:A:LEU:H | 7 | 0.11 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD11 | 11 | 0.11 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD12 | 11 | 0.11 |
| (1,478) | 1:77:A:LEU:H | 1:77:A:LEU:HD13 | 11 | 0.11 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB1 | 9 | 0.11 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB2 | 9 | 0.11 |
| (1,470) | 1:71:A:ALA:H | 1:74:A:ALA:HB3 | 9 | 0.11 |
| (1,350) | 1:47:A:LEU:HD11 | 1:48:A:ILE:H | 4 | 0.11 |
| (1,350) | 1:47:A:LEU:HD12 | 1:48:A:ILE:H | 4 | 0.11 |
| (1,350) | 1:47:A:LEU:HD13 | 1:48:A:ILE:H | 4 | 0.11 |
| (1,345) | 1:48:A:ILE:H | 1:48:A:ILE:HG21 | 20 | 0.11 |
| (1,345) | 1:48:A:ILE:H | 1:48:A:ILE:HG22 | 20 | 0.11 |
| (1,345) | 1:48:A:ILE:H | 1:48:A:ILE:HG23 | 20 | 0.11 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 5 | 0.11 |
| (1,309) | 1:32:A:ASP:H | 1:32:A:ASP:HB3 | 17 | 0.11 |
| (1,267) | 1:27:A:ARG:HG3 | 1:28:A:VAL:H | 8 | 0.11 |
| (1,202) | 1:15:A:LEU:HB3 | 1:16:A:CYS:H | 18 | 0.11 |
| (1,199) | 1:13:A:LYS:HB2 | 1:14:A:VAL:H | 8 | 0.11 |
| (1,199) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 8 | 0.11 |
| (1,184) | 1:22:A:ILE:HD11 | 1:23:A:LEU:H | 1 | 0.11 |
| (1,184) | 1:22:A:ILE:HD12 | 1:23:A:LEU:H | 1 | 0.11 |
| (1,184) | 1:22:A:ILE:HD13 | 1:23:A:LEU:H | 1 | 0.11 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 10 | 0.11 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 10 | 0.11 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 10 | 0.11 |
| (1,138) | 1:11:A:THR:HG21 | 1:15:A:LEU:HG | 18 | 0.11 |
| (1,138) | 1:11:A:THR:HG22 | 1:15:A:LEU:HG | 18 | 0.11 |
| (1,138) | 1:11:A:THR:HG23 | 1:15:A:LEU:HG | 18 | 0.11 |
| (1,74) | 1:50:A:ARG:HA | 1:50:A:ARG:HD2 | 2 | 0.11 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD21 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD22 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD11 | 1:64:A:LEU:HD23 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD21 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD22 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD12 | 1:64:A:LEU:HD23 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD21 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD22 | 8 | 0.11 |
| (1,62) | 1:51:A:ILE:HD13 | 1:64:A:LEU:HD23 | 8 | 0.11 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG21 | 5 | 0.11 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG22 | 5 | 0.11 |
| (1,37) | 1:31:A:ASP:HB2 | 1:69:A:THR:HG23 | 5 | 0.11 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG11 | 12 | 0.11 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG12 | 12 | 0.11 |
| (1,24) | 1:12:A:GLU:HG3 | 1:30:A:VAL:HG13 | 12 | 0.11 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 3 | 0.11 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 3 | 0.11 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 3 | 0.11 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD11 | 11 | 0.1 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD12 | 11 | 0.1 |
| (1,952) | 1:19:A:TYR:HE1 | 1:51:A:ILE:HD13 | 11 | 0.1 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD11 | 11 | 0.1 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD12 | 11 | 0.1 |
| (1,952) | 1:19:A:TYR:HE2 | 1:51:A:ILE:HD13 | 11 | 0.1 |
| (1,930) | 1:13:A:LYS:HB3 | 1:14:A:VAL:H | 3 | 0.1 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD21 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD22 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD11 | 1:43:A:LEU:HD23 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD21 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD22 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD12 | 1:43:A:LEU:HD23 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD21 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD22 | 13 | 0.1 |
| (1,824) | 1:22:A:ILE:HD13 | 1:43:A:LEU:HD23 | 13 | 0.1 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD11 | 11 | 0.1 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD12 | 11 | 0.1 |
| (1,799) | 1:11:A:THR:HA | 1:55:A:LEU:HD13 | 11 | 0.1 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD11 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD12 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB1 | 1:64:A:LEU:HD13 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD11 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD12 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB2 | 1:64:A:LEU:HD13 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD11 | 1 | 0.1 |
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD12 | 1 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,759) | 1:44:A:ALA:HB3 | 1:64:A:LEU:HD13 | 1 | 0.1 |
| (1,447) | 1:62:A:ARG:HB3 | 1:63:A:GLN:H | 1 | 0.1 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 10 | 0.1 |
| (1,422) | 1:55:A:LEU:HB3 | 1:57:A:VAL:H | 13 | 0.1 |
| (1,395) | 1:51:A:ILE:HG21 | 1:54:A:GLU:H | 8 | 0.1 |
| (1,395) | 1:51:A:ILE:HG22 | 1:54:A:GLU:H | 8 | 0.1 |
| (1,395) | 1:51:A:ILE:HG23 | 1:54:A:GLU:H | 8 | 0.1 |
| (1,373) | 1:53:A:GLU:H | 1:53:A:GLU:HG3 | 16 | 0.1 |
| (1,373) | 1:53:A:GLU:H | 1:53:A:GLU:HG3 | 17 | 0.1 |
| (1,370) | 1:50:A:ARG:HB2 | 1:51:A:ILE:H | 20 | 0.1 |
| (1,326) | 1:47:A:LEU:HB2 | 1:48:A:ILE:H | 17 | 0.1 |
| (1,248) | 1:21:A:GLU:HG3 | 1:22:A:ILE:H | 17 | 0.1 |
| (1,196) | 1:13:A:LYS:H | 1:13:A:LYS:HG3 | 10 | 0.1 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD11 | 19 | 0.1 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD12 | 19 | 0.1 |
| (1,179) | 1:13:A:LYS:H | 1:15:A:LEU:HD13 | 19 | 0.1 |
| (1,123) | 1:20:A:ALA:HA | 1:28:A:VAL:HG11 | 4 | 0.1 |
| (1,123) | 1:20:A:ALA:HA | 1:28:A:VAL:HG12 | 4 | 0.1 |
| (1,123) | 1:20:A:ALA:HA | 1:28:A:VAL:HG13 | 4 | 0.1 |
| (1,105) | 1:51:A:ILE:HD11 | 1:59:A:LEU:HG | 2 | 0.1 |
| (1,105) | 1:51:A:ILE:HD12 | 1:59:A:LEU:HG | 2 | 0.1 |
| (1,105) | 1:51:A:ILE:HD13 | 1:59:A:LEU:HG | 2 | 0.1 |
| (1,95) | 1:14:A:VAL:HG11 | 1:54:A:GLU:HB2 | 13 | 0.1 |
| (1,95) | 1:14:A:VAL:HG12 | 1:54:A:GLU:HB2 | 13 | 0.1 |
| (1,95) | 1:14:A:VAL:HG13 | 1:54:A:GLU:HB2 | 13 | 0.1 |
| (1,11) | 1:23:A:LEU:HD11 | 1:39:A:GLY:HA3 | 9 | 0.1 |
| (1,11) | 1:23:A:LEU:HD12 | 1:39:A:GLY:HA3 | 9 | 0.1 |
| (1,11) | 1:23:A:LEU:HD13 | 1:39:A:GLY:HA3 | 9 | 0.1 |

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

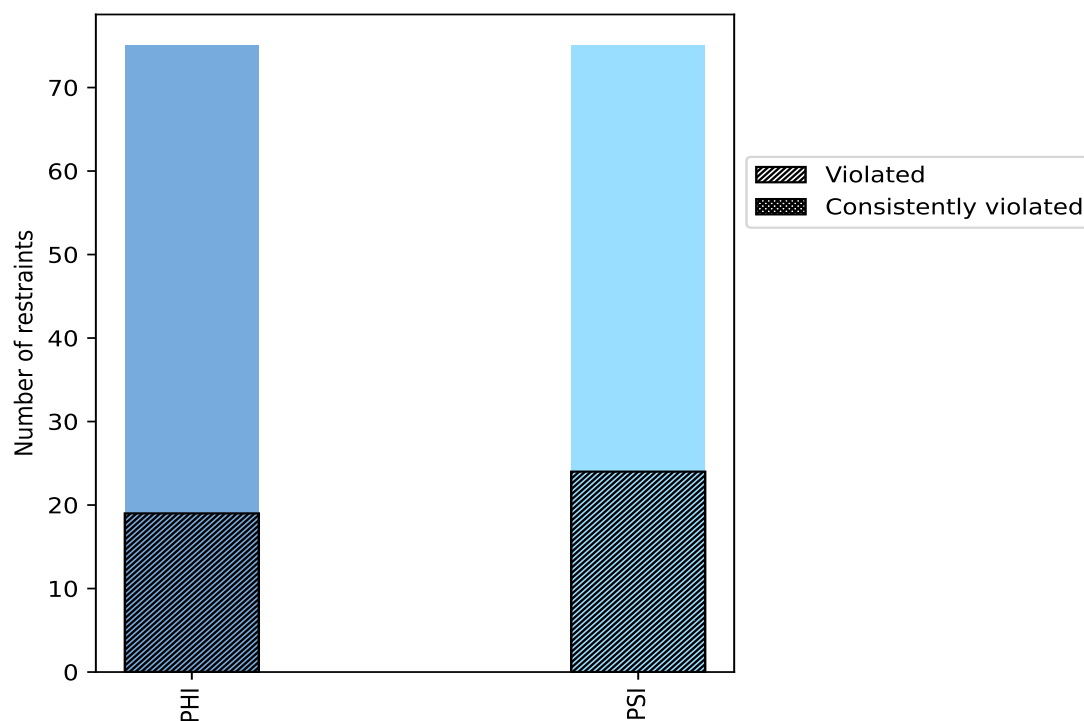
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 75 | 50.0 | 19 | 25.3 | 12.7 | 0 | 0.0 | 0.0 |
| PSI | 75 | 50.0 | 24 | 32.0 | 16.0 | 0 | 0.0 | 0.0 |
| Total | 150 | 100.0 | 43 | 28.7 | 28.7 | 0 | 0.0 | 0.0 |

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

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



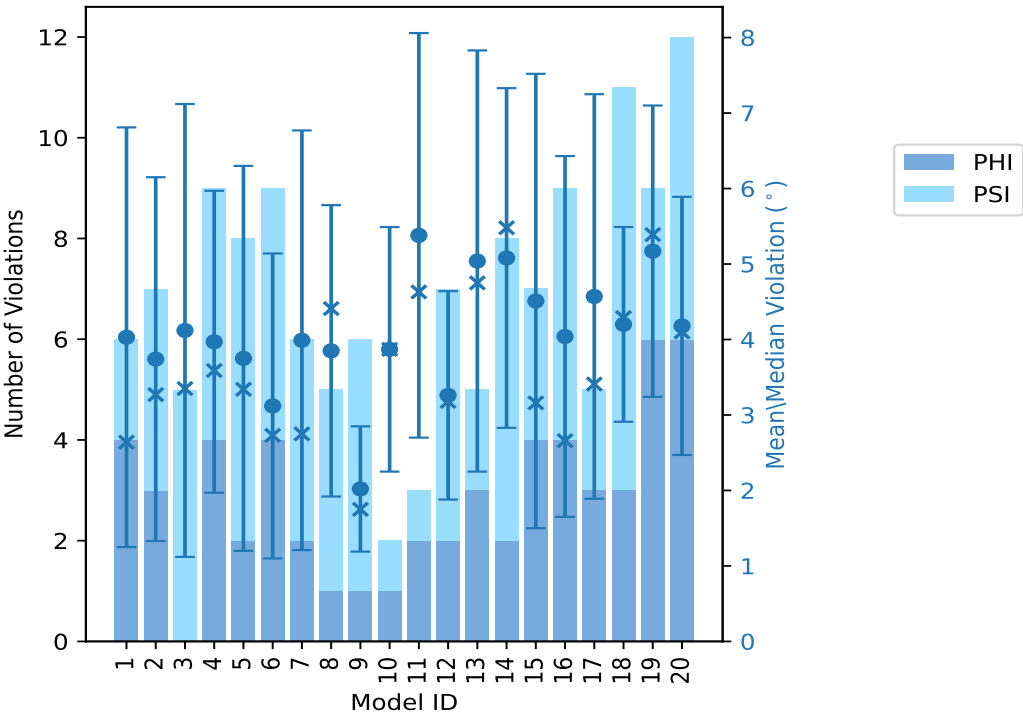
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 4 | 2 | 6 | 4.03 | 9.49 | 2.78 | 2.64 |
| 2 | 3 | 4 | 7 | 3.74 | 8.99 | 2.41 | 3.27 |
| 3 | 0 | 5 | 5 | 4.12 | 9.76 | 3.0 | 3.35 |
| 4 | 4 | 5 | 9 | 3.97 | 8.21 | 2.0 | 3.59 |
| 5 | 2 | 6 | 8 | 3.75 | 9.83 | 2.55 | 3.34 |
| 6 | 4 | 5 | 9 | 3.12 | 8.5 | 2.02 | 2.73 |
| 7 | 2 | 4 | 6 | 3.99 | 9.82 | 2.78 | 2.75 |
| 8 | 1 | 4 | 5 | 3.85 | 6.65 | 1.93 | 4.41 |
| 9 | 1 | 5 | 6 | 2.02 | 3.63 | 0.83 | 1.75 |
| 10 | 1 | 1 | 2 | 3.87 | 5.49 | 1.62 | 3.87 |
| 11 | 2 | 1 | 3 | 5.38 | 8.97 | 2.68 | 4.63 |
| 12 | 2 | 5 | 7 | 3.26 | 5.7 | 1.38 | 3.18 |
| 13 | 3 | 2 | 5 | 5.04 | 9.28 | 2.79 | 4.75 |
| 14 | 2 | 6 | 8 | 5.08 | 7.9 | 2.25 | 5.48 |
| 15 | 4 | 3 | 7 | 4.51 | 9.53 | 3.01 | 3.16 |
| 16 | 4 | 5 | 9 | 4.04 | 9.22 | 2.39 | 2.66 |
| 17 | 3 | 2 | 5 | 4.57 | 9.82 | 2.68 | 3.41 |
| 18 | 3 | 8 | 11 | 4.2 | 7.17 | 1.29 | 4.29 |
| 19 | 6 | 3 | 9 | 5.17 | 7.99 | 1.93 | 5.39 |
| 20 | 6 | 6 | 12 | 4.18 | 6.64 | 1.71 | 4.1 |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

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

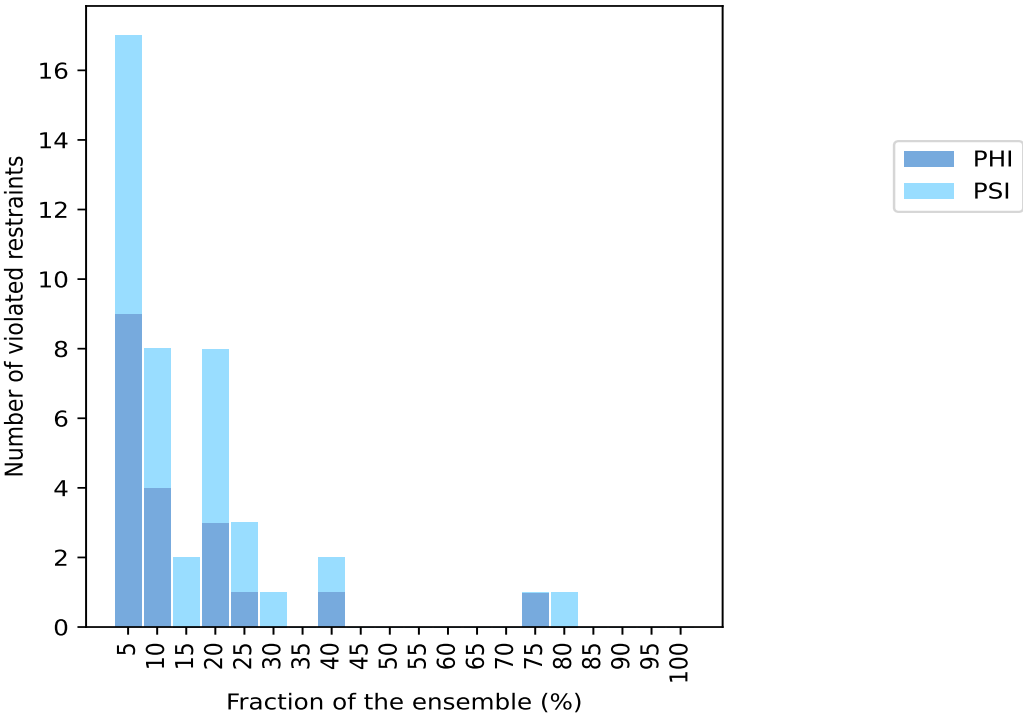
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 |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

¹ Number of models with violations

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

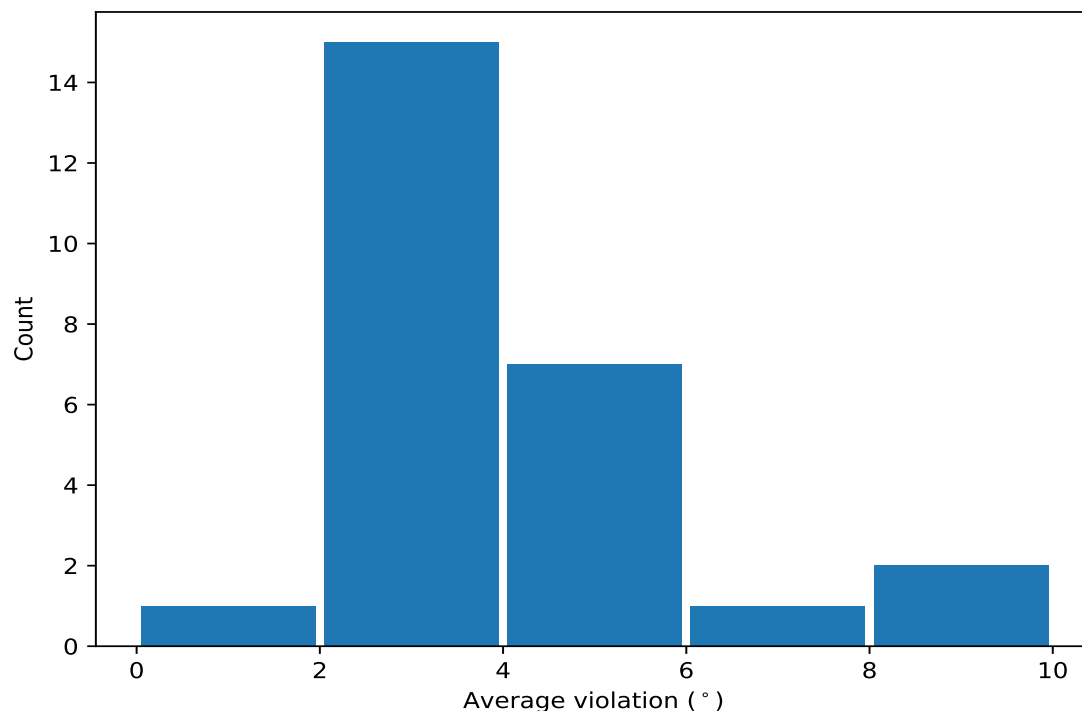


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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 |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 16 | 3.69 | 1.36 | 3.4 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 15 | 5.21 | 2.62 | 4.78 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 8 | 3.57 | 1.18 | 3.2 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 8 | 3.3 | 1.54 | 3.38 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 6 | 2.74 | 1.13 | 2.6 |
| (1,147) | 1:85:A:SER:C | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 5 | 8.44 | 2.18 | 9.49 |
| (1,144) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ALA:N | 5 | 3.51 | 1.81 | 3.27 |
| (1,76) | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1:45:A:MET:N | 5 | 3.04 | 1.84 | 2.46 |
| (1,149) | 1:88:A:GLN:C | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 4 | 7.89 | 1.82 | 8.75 |
| (1,36) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C | 1:22:A:ILE:N | 4 | 5.6 | 2.41 | 6.02 |
| (1,2) | 1:3:A:MET:N | 1:3:A:MET:CA | 1:3:A:MET:C | 1:4:A:ALA:N | 4 | 4.57 | 1.94 | 4.28 |
| (1,124) | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 1:72:A:GLY:N | 4 | 4.11 | 2.5 | 3.68 |
| (1,43) | 1:24:A:GLY:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 4 | 3.94 | 3.05 | 2.27 |
| (1,131) | 1:74:A:ALA:C | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 4 | 2.56 | 1.63 | 1.82 |
| (1,12) | 1:9:A:SER:N | 1:9:A:SER:CA | 1:9:A:SER:C | 1:10:A:ALA:N | 4 | 2.21 | 0.53 | 2.08 |
| (1,92) | 1:52:A:ARG:N | 1:52:A:ARG:CA | 1:52:A:ARG:C | 1:53:A:GLU:N | 4 | 1.79 | 0.28 | 1.87 |
| (1,58) | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 1:33:A:ALA:N | 3 | 4.81 | 2.15 | 4.16 |
| (1,56) | 1:31:A:ASP:N | 1:31:A:ASP:CA | 1:31:A:ASP:C | 1:32:A:ASP:N | 3 | 2.51 | 1.42 | 2.0 |
| (1,150) | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 1:90:A:GLU:N | 2 | 8.2 | 1.55 | 8.2 |
| (1,20) | 1:13:A:LYS:N | 1:13:A:LYS:CA | 1:13:A:LYS:C | 1:14:A:VAL:N | 2 | 5.46 | 0.68 | 5.46 |

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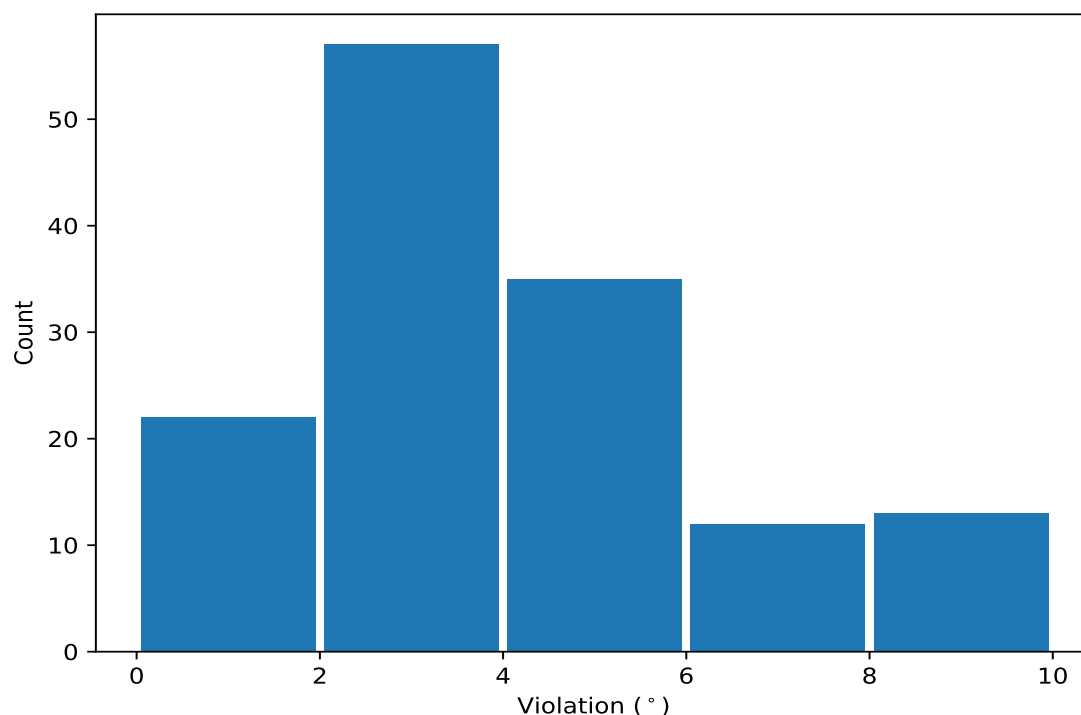
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,128) | 1:73:A:VAL:N | 1:73:A:VAL:CA | 1:73:A:VAL:C | 1:74:A:ALA:N | 2 | 4.12 | 1.8 | 4.12 |
| (1,135) | 1:76:A:ALA:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 2 | 3.97 | 1.42 | 3.97 |
| (1,15) | 1:10:A:ALA:C | 1:11:A:THR:N | 1:11:A:THR:CA | 1:11:A:THR:C | 2 | 3.07 | 0.12 | 3.07 |
| (1,9) | 1:7:A:PRO:C | 1:8:A:GLU:N | 1:8:A:GLU:CA | 1:8:A:GLU:C | 2 | 2.92 | 0.17 | 2.92 |
| (1,57) | 1:31:A:ASP:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 2 | 2.84 | 1.66 | 2.84 |
| (1,74) | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 1:44:A:ALA:N | 2 | 2.71 | 0.56 | 2.71 |

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 (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 5 | 9.83 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,147) | 1:85:A:SER:C | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 7 | 9.82 |
| (1,147) | 1:85:A:SER:C | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 17 | 9.82 |
| (1,150) | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 1:90:A:GLU:N | 3 | 9.76 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 15 | 9.53 |
| (1,147) | 1:85:A:SER:C | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 1 | 9.49 |
| (1,149) | 1:88:A:GLN:C | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 13 | 9.28 |
| (1,43) | 1:24:A:GLY:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 16 | 9.22 |
| (1,149) | 1:88:A:GLN:C | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 2 | 8.99 |
| (1,147) | 1:85:A:SER:C | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 11 | 8.97 |
| (1,149) | 1:88:A:GLN:C | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 15 | 8.52 |
| (1,36) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C | 1:22:A:ILE:N | 6 | 8.5 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 4 | 8.21 |
| (1,141) | 1:79:A:ALA:C | 1:80:A:LYS:N | 1:80:A:LYS:CA | 1:80:A:LYS:C | 19 | 7.99 |
| (1,124) | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 1:72:A:GLY:N | 19 | 7.98 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 14 | 7.9 |
| (1,58) | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 1:33:A:ALA:N | 14 | 7.7 |
| (1,2) | 1:3:A:MET:N | 1:3:A:MET:CA | 1:3:A:MET:C | 1:4:A:ALA:N | 18 | 7.17 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 13 | 6.95 |
| (1,144) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ALA:N | 14 | 6.89 |
| (1,150) | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 1:90:A:GLU:N | 8 | 6.65 |
| (1,76) | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1:45:A:MET:N | 20 | 6.64 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 20 | 6.61 |
| (1,36) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C | 1:22:A:ILE:N | 16 | 6.43 |
| (1,20) | 1:13:A:LYS:N | 1:13:A:LYS:CA | 1:13:A:LYS:C | 1:14:A:VAL:N | 20 | 6.14 |
| (1,128) | 1:73:A:VAL:N | 1:73:A:VAL:CA | 1:73:A:VAL:C | 1:74:A:ALA:N | 14 | 5.93 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 19 | 5.73 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 1 | 5.7 |
| (1,2) | 1:3:A:MET:N | 1:3:A:MET:CA | 1:3:A:MET:C | 1:4:A:ALA:N | 12 | 5.7 |
| (1,13) | 1:9:A:SER:C | 1:10:A:ALA:N | 1:10:A:ALA:CA | 1:10:A:ALA:C | 4 | 5.68 |
| (1,36) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C | 1:22:A:ILE:N | 18 | 5.61 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 10 | 5.49 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 19 | 5.41 |
| (1,135) | 1:76:A:ALA:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 19 | 5.39 |
| (1,73) | 1:42:A:ALA:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 4 | 5.37 |
| (1,131) | 1:74:A:ALA:C | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 20 | 5.31 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 20 | 5.21 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 14 | 5.02 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 19 | 4.99 |
| (1,35) | 1:20:A:ALA:C | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C | 18 | 4.93 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 16 | 4.78 |
| (1,149) | 1:88:A:GLN:C | 1:89:A:PHE:N | 1:89:A:PHE:CA | 1:89:A:PHE:C | 7 | 4.77 |
| (1,20) | 1:13:A:LYS:N | 1:13:A:LYS:CA | 1:13:A:LYS:C | 1:14:A:VAL:N | 8 | 4.77 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 16 | 4.76 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 13 | 4.75 |
| (1,14) | 1:10:A:ALA:N | 1:10:A:ALA:CA | 1:10:A:ALA:C | 1:11:A:THR:N | 12 | 4.69 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 11 | 4.63 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 5 | 4.54 |
| (1,57) | 1:31:A:ASP:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 18 | 4.5 |
| (1,56) | 1:31:A:ASP:N | 1:31:A:ASP:CA | 1:31:A:ASP:C | 1:32:A:ASP:N | 2 | 4.45 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 8 | 4.41 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 18 | 4.36 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 15 | 4.33 |
| (1,24) | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 1:16:A:CYS:N | 18 | 4.29 |
| (1,124) | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 1:72:A:GLY:N | 20 | 4.21 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 17 | 4.17 |
| (1,58) | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 1:33:A:ALA:N | 3 | 4.16 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 2 | 4.13 |
| (1,147) | 1:85:A:SER:C | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 19 | 4.12 |
| (1,142) | 1:80:A:LYS:N | 1:80:A:LYS:CA | 1:80:A:LYS:C | 1:81:A:SER:N | 4 | 4.12 |
| (1,101) | 1:56:A:GLY:C | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 20 | 3.98 |
| (1,112) | 1:63:A:GLN:N | 1:63:A:GLN:CA | 1:63:A:GLN:C | 1:64:A:LEU:N | 5 | 3.78 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 5 | 3.73 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 9 | 3.63 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 4 | 3.59 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 6 | 3.53 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 18 | 3.44 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 17 | 3.41 |
| (1,144) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ALA:N | 3 | 3.35 |
| (1,144) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ALA:N | 2 | 3.27 |
| (1,74) | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 1:44:A:ALA:N | 19 | 3.27 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 18 | 3.22 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 6 | 3.2 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 12 | 3.18 |
| (1,15) | 1:10:A:ALA:C | 1:11:A:THR:N | 1:11:A:THR:CA | 1:11:A:THR:C | 12 | 3.18 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 15 | 3.16 |
| (1,124) | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 1:72:A:GLY:N | 18 | 3.14 |
| (1,9) | 1:7:A:PRO:C | 1:8:A:GLU:N | 1:8:A:GLU:CA | 1:8:A:GLU:C | 18 | 3.09 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1 | 3.03 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 15 | 3.0 |
| (1,12) | 1:9:A:SER:N | 1:9:A:SER:CA | 1:9:A:SER:C | 1:10:A:ALA:N | 7 | 2.98 |
| (1,136) | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 1:78:A:ALA:N | 5 | 2.96 |
| (1,15) | 1:10:A:ALA:C | 1:11:A:THR:N | 1:11:A:THR:CA | 1:11:A:THR:C | 20 | 2.95 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 17 | 2.87 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 14 | 2.87 |
| (1,2) | 1:3:A:MET:N | 1:3:A:MET:CA | 1:3:A:MET:C | 1:4:A:ALA:N | 6 | 2.85 |
| (1,137) | 1:77:A:LEU:C | 1:78:A:ALA:N | 1:78:A:ALA:CA | 1:78:A:ALA:C | 5 | 2.78 |
| (1,9) | 1:7:A:PRO:C | 1:8:A:GLU:N | 1:8:A:GLU:CA | 1:8:A:GLU:C | 12 | 2.75 |
| (1,66) | 1:37:A:LEU:N | 1:37:A:LEU:CA | 1:37:A:LEU:C | 1:38:A:GLY:N | 6 | 2.73 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 16 | 2.66 |
| (1,76) | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1:45:A:MET:N | 16 | 2.65 |
| (1,58) | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 1:33:A:ALA:N | 17 | 2.56 |
| (1,135) | 1:76:A:ALA:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 4 | 2.55 |
| (1,2) | 1:3:A:MET:N | 1:3:A:MET:CA | 1:3:A:MET:C | 1:4:A:ALA:N | 20 | 2.54 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 11 | 2.53 |
| (1,144) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ALA:N | 7 | 2.52 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 20 | 2.47 |
| (1,76) | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1:45:A:MET:N | 9 | 2.46 |
| (1,148) | 1:86:A:HIS:N | 1:86:A:HIS:CA | 1:86:A:HIS:C | 1:87:A:PRO:N | 18 | 2.45 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 20 | 2.44 |
| (1,12) | 1:9:A:SER:N | 1:9:A:SER:CA | 1:9:A:SER:C | 1:10:A:ALA:N | 4 | 2.42 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 16 | 2.33 |
| (1,128) | 1:73:A:VAL:N | 1:73:A:VAL:CA | 1:73:A:VAL:C | 1:74:A:ALA:N | 16 | 2.32 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,43) | 1:24:A:GLY:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 14 | 2.29 |
| (1,131) | 1:74:A:ALA:C | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 1 | 2.26 |
| (1,43) | 1:24:A:GLY:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 10 | 2.25 |
| (1,132) | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 1:76:A:ALA:N | 7 | 2.23 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 3 | 2.22 |
| (1,123) | 1:70:A:PRO:C | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 13 | 2.2 |
| (1,143) | 1:80:A:LYS:C | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 6 | 2.19 |
| (1,74) | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 1:44:A:ALA:N | 8 | 2.15 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 2 | 2.11 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 2 | 2.11 |
| (1,92) | 1:52:A:ARG:N | 1:52:A:ARG:CA | 1:52:A:ARG:C | 1:53:A:GLU:N | 14 | 2.07 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 13 | 2.01 |
| (1,43) | 1:24:A:GLY:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 6 | 2.01 |
| (1,56) | 1:31:A:ASP:N | 1:31:A:ASP:CA | 1:31:A:ASP:C | 1:32:A:ASP:N | 1 | 2.0 |
| (1,92) | 1:52:A:ARG:N | 1:52:A:ARG:CA | 1:52:A:ARG:C | 1:53:A:GLU:N | 4 | 1.99 |
| (1,36) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C | 1:22:A:ILE:N | 4 | 1.84 |
| (1,76) | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1:45:A:MET:N | 12 | 1.82 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 9 | 1.76 |
| (1,92) | 1:52:A:ARG:N | 1:52:A:ARG:CA | 1:52:A:ARG:C | 1:53:A:GLU:N | 6 | 1.75 |
| (1,12) | 1:9:A:SER:N | 1:9:A:SER:CA | 1:9:A:SER:C | 1:10:A:ALA:N | 9 | 1.74 |
| (1,12) | 1:9:A:SER:N | 1:9:A:SER:CA | 1:9:A:SER:C | 1:10:A:ALA:N | 1 | 1.7 |
| (1,76) | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1:45:A:MET:N | 15 | 1.63 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 7 | 1.62 |
| (1,21) | 1:13:A:LYS:C | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C | 20 | 1.62 |
| (1,55) | 1:30:A:VAL:C | 1:31:A:ASP:N | 1:31:A:ASP:CA | 1:31:A:ASP:C | 19 | 1.61 |
| (1,144) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ALA:N | 12 | 1.52 |
| (1,131) | 1:74:A:ALA:C | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 15 | 1.37 |
| (1,92) | 1:52:A:ARG:N | 1:52:A:ARG:CA | 1:52:A:ARG:C | 1:53:A:GLU:N | 9 | 1.36 |
| (1,30) | 1:18:A:LEU:N | 1:18:A:LEU:CA | 1:18:A:LEU:C | 1:19:A:TYR:N | 5 | 1.31 |
| (1,131) | 1:74:A:ALA:C | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 6 | 1.3 |
| (1,37) | 1:21:A:GLU:C | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 8 | 1.26 |
| (1,57) | 1:31:A:ASP:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 16 | 1.19 |
| (1,90) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:ARG:N | 9 | 1.16 |
| (1,108) | 1:61:A:ILE:N | 1:61:A:ILE:CA | 1:61:A:ILE:C | 1:62:A:ARG:N | 3 | 1.12 |
| (1,124) | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C | 1:72:A:GLY:N | 2 | 1.09 |
| (1,56) | 1:31:A:ASP:N | 1:31:A:ASP:CA | 1:31:A:ASP:C | 1:32:A:ASP:N | 5 | 1.09 |