



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 10:29 AM EST

PDB ID : 6E9M
BMRB ID : 30505
Title : Solution NMR Structure of a Class I Hydrophobin from *Wallemia ichthyophaga*
Authors : Kenward, C.; Langelaan, D.N.
Deposited on : 2018-08-01

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

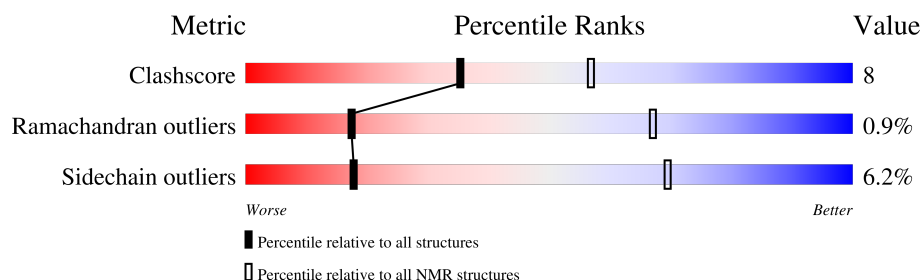
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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 | 90 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:4-A:32, A:44-A:88 (74) | 0.71 | 17 |

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1291 atoms, of which 638 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrophobin.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 90 | Total | C | H | N | O | S | 0 |
| | | | 1291 | 397 | 638 | 107 | 141 | 8 | |

There are 2 discrepancies between the modelled and reference sequences:

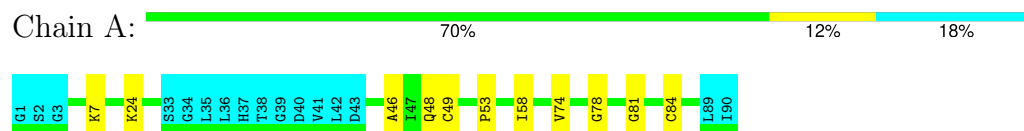
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1 | GLY | - | expression tag | UNP R9A9N7 |
| A | 2 | SER | - | expression tag | UNP R9A9N7 |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Hydrophobin

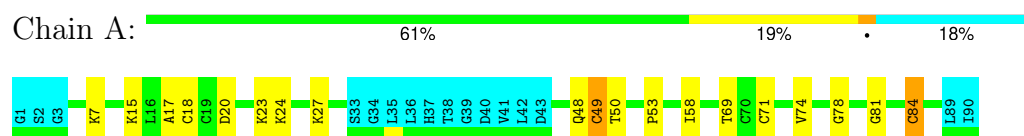


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

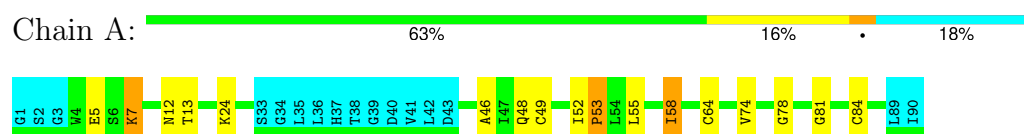
4.2.1 Score per residue for model 1

- Molecule 1: Hydrophobin



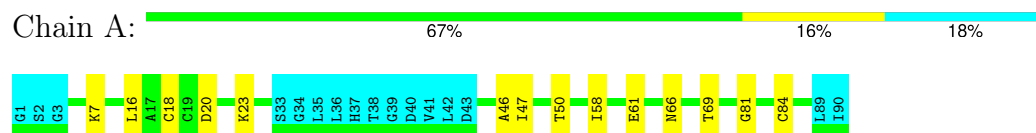
4.2.2 Score per residue for model 2

- Molecule 1: Hydrophobin



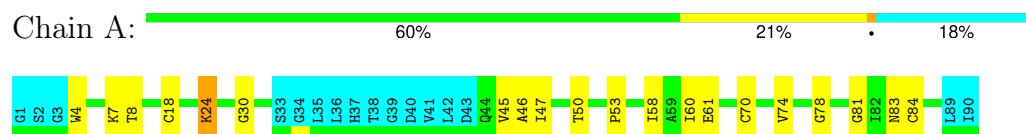
4.2.3 Score per residue for model 3

- Molecule 1: Hydrophobin



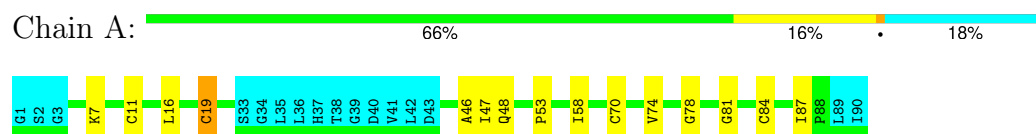
4.2.4 Score per residue for model 4

- Molecule 1: Hydrophobin



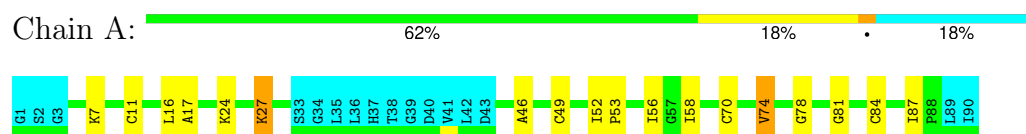
4.2.5 Score per residue for model 5

- Molecule 1: Hydrophobin



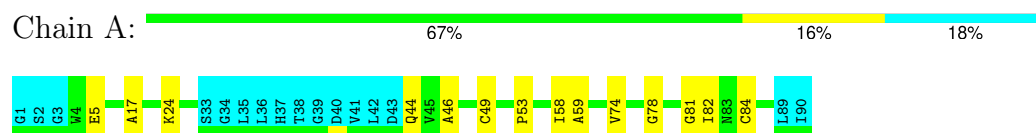
4.2.6 Score per residue for model 6

- Molecule 1: Hydrophobin



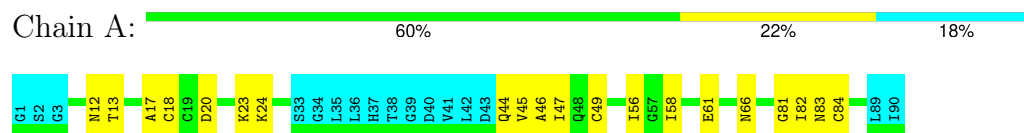
4.2.7 Score per residue for model 7

- Molecule 1: Hydrophobin



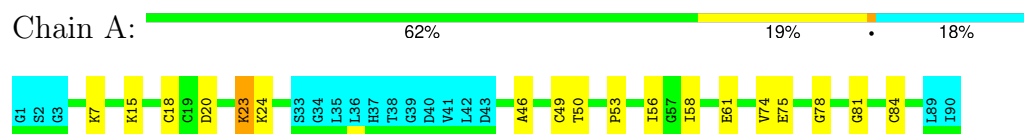
4.2.8 Score per residue for model 8

- Molecule 1: Hydrophobin



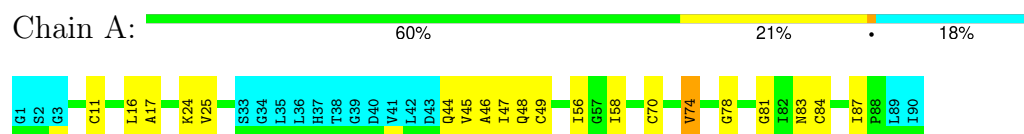
4.2.9 Score per residue for model 9

- Molecule 1: Hydrophobin



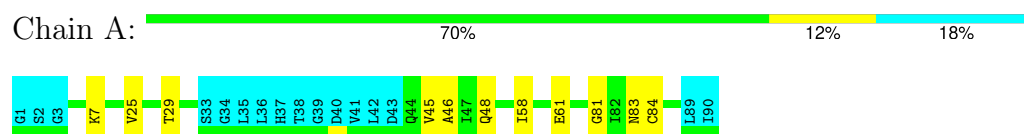
4.2.10 Score per residue for model 10

- Molecule 1: Hydrophobin



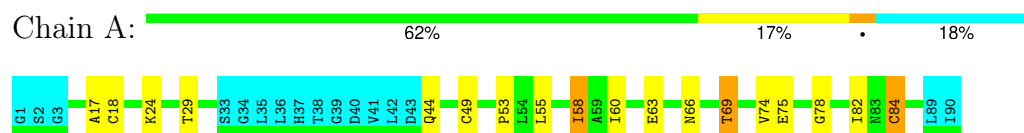
4.2.11 Score per residue for model 11

- Molecule 1: Hydrophobin



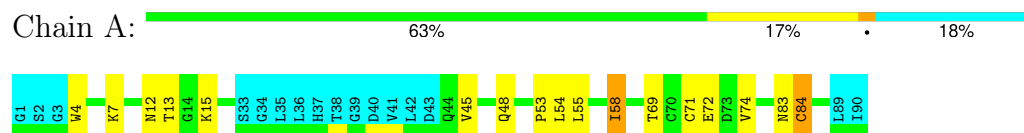
4.2.12 Score per residue for model 12

- Molecule 1: Hydrophobin



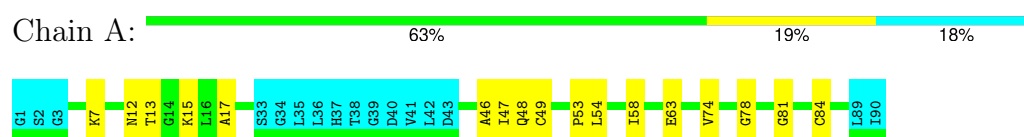
4.2.13 Score per residue for model 13

- Molecule 1: Hydrophobin



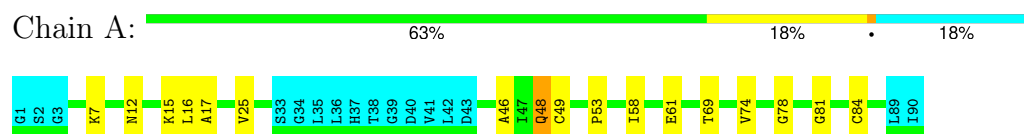
4.2.14 Score per residue for model 14

- Molecule 1: Hydrophobin



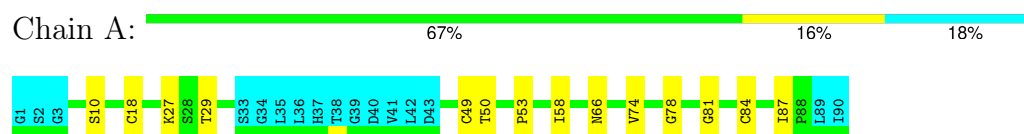
4.2.15 Score per residue for model 15

- Molecule 1: Hydrophobin



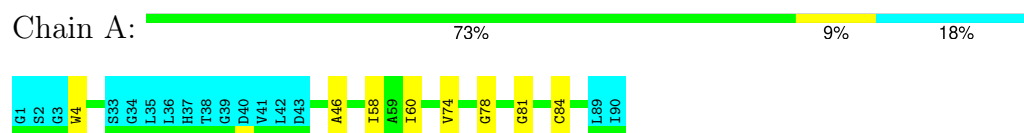
4.2.16 Score per residue for model 16

- Molecule 1: Hydrophobin



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Hydrophobin



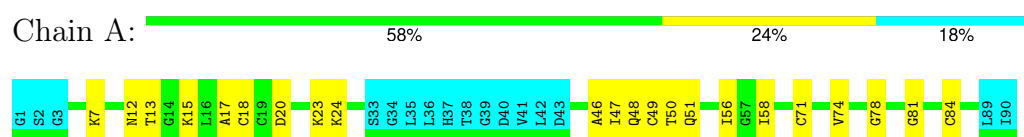
4.2.18 Score per residue for model 18

- Molecule 1: Hydrophobin



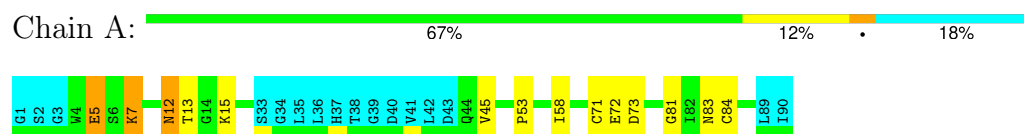
4.2.19 Score per residue for model 19

- Molecule 1: Hydrophobin



4.2.20 Score per residue for model 20

- Molecule 1: Hydrophobin



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| ARIA | refinement | 2.3.1 |
| ARIA | structure calculation | 2.3.1 |

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

| Chemical shift file(s) | working_cs.cif |
|--|----------------|
| Number of chemical shift lists | 1 |
| Total number of shifts | 1013 |
| Number of shifts mapped to atoms | 1013 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 92% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 544 | 527 | 527 | 8±2 |
| All | All | 10880 | 10540 | 10540 | 166 |

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 8.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:LEU:HG | 1:A:70:CYS:SG | 0.75 | 2.21 | 10 | 3 |
| 1:A:69:THR:HB | 1:A:84:CYS:SG | 0.74 | 2.22 | 12 | 3 |
| 1:A:18:CYS:SG | 1:A:66:ASN:HB2 | 0.73 | 2.24 | 3 | 1 |
| 1:A:11:CYS:SG | 1:A:87:ILE:HG21 | 0.66 | 2.31 | 5 | 3 |
| 1:A:81:GLY:HA3 | 1:A:84:CYS:SG | 0.64 | 2.33 | 9 | 17 |
| 1:A:45:VAL:HG12 | 1:A:83:ASN:HA | 0.61 | 1.72 | 11 | 6 |
| 1:A:19:CYS:SG | 1:A:47:ILE:HG13 | 0.61 | 2.35 | 5 | 1 |
| 1:A:49:CYS:HB3 | 1:A:78:GLY:O | 0.58 | 1.97 | 7 | 7 |
| 1:A:45:VAL:CG1 | 1:A:83:ASN:HA | 0.55 | 2.31 | 8 | 1 |
| 1:A:46:ALA:HA | 1:A:81:GLY:O | 0.54 | 2.02 | 14 | 15 |
| 1:A:17:ALA:HB1 | 1:A:49:CYS:SG | 0.54 | 2.43 | 6 | 9 |
| 1:A:15:LYS:HB2 | 1:A:71:CYS:O | 0.53 | 2.04 | 18 | 3 |
| 1:A:10:SER:OG | 1:A:87:ILE:HB | 0.52 | 2.03 | 16 | 1 |
| 1:A:55:LEU:O | 1:A:58:ILE:HB | 0.51 | 2.05 | 2 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:25:VAL:HG22 | 1:A:48:GLN:NE2 | 0.51 | 2.19 | 15 | 2 |
| 1:A:20:ASP:HB3 | 1:A:23:LYS:HB2 | 0.51 | 1.81 | 9 | 5 |
| 1:A:69:THR:CB | 1:A:84:CYS:SG | 0.51 | 2.98 | 1 | 2 |
| 1:A:12:ASN:HD22 | 1:A:13:THR:N | 0.50 | 2.03 | 20 | 1 |
| 1:A:5:GLU:OE1 | 1:A:59:ALA:HA | 0.50 | 2.07 | 7 | 1 |
| 1:A:18:CYS:HB3 | 1:A:50:THR:O | 0.49 | 2.06 | 3 | 1 |
| 1:A:15:LYS:HD3 | 1:A:74:VAL:HG23 | 0.49 | 1.83 | 9 | 4 |
| 1:A:15:LYS:NZ | 1:A:73:ASP:HA | 0.49 | 2.22 | 20 | 1 |
| 1:A:18:CYS:HB2 | 1:A:50:THR:O | 0.49 | 2.08 | 16 | 5 |
| 1:A:20:ASP:CB | 1:A:23:LYS:HD3 | 0.49 | 2.38 | 19 | 1 |
| 1:A:56:ILE:HD12 | 1:A:56:ILE:H | 0.48 | 1.67 | 8 | 4 |
| 1:A:18:CYS:HB3 | 1:A:66:ASN:HB2 | 0.48 | 1.85 | 16 | 3 |
| 1:A:70:CYS:SG | 1:A:87:ILE:HD13 | 0.47 | 2.49 | 10 | 1 |
| 1:A:74:VAL:CG1 | 1:A:78:GLY:HA2 | 0.46 | 2.40 | 9 | 12 |
| 1:A:44:GLN:HA | 1:A:83:ASN:OD1 | 0.46 | 2.11 | 10 | 1 |
| 1:A:49:CYS:HB2 | 1:A:78:GLY:O | 0.46 | 2.11 | 9 | 3 |
| 1:A:4:TRP:CD2 | 1:A:60:ILE:HB | 0.46 | 2.46 | 17 | 2 |
| 1:A:44:GLN:HB3 | 1:A:82:ILE:HG23 | 0.45 | 1.87 | 8 | 3 |
| 1:A:71:CYS:N | 1:A:84:CYS:SG | 0.45 | 2.89 | 1 | 2 |
| 1:A:5:GLU:OE2 | 1:A:7:LYS:HD2 | 0.45 | 2.12 | 20 | 1 |
| 1:A:25:VAL:HG22 | 1:A:48:GLN:OE1 | 0.45 | 2.11 | 10 | 2 |
| 1:A:47:ILE:HD11 | 1:A:84:CYS:HB2 | 0.45 | 1.88 | 14 | 2 |
| 1:A:27:LYS:HE2 | 1:A:27:LYS:HA | 0.45 | 1.88 | 1 | 1 |
| 1:A:4:TRP:CZ2 | 1:A:54:LEU:HD22 | 0.44 | 2.47 | 13 | 1 |
| 1:A:15:LYS:HD3 | 1:A:74:VAL:HG13 | 0.44 | 1.88 | 15 | 1 |
| 1:A:12:ASN:OD1 | 1:A:13:THR:HG23 | 0.44 | 2.13 | 8 | 4 |
| 1:A:29:THR:HB | 1:A:75:GLU:OE2 | 0.43 | 2.13 | 12 | 1 |
| 1:A:20:ASP:HB3 | 1:A:23:LYS:CB | 0.43 | 2.43 | 9 | 1 |
| 1:A:20:ASP:OD1 | 1:A:23:LYS:HB2 | 0.43 | 2.14 | 9 | 1 |
| 1:A:54:LEU:HA | 1:A:63:GLU:OE1 | 0.43 | 2.12 | 14 | 1 |
| 1:A:24:LYS:HD3 | 1:A:47:ILE:HG22 | 0.43 | 1.89 | 10 | 1 |
| 1:A:74:VAL:HG12 | 1:A:78:GLY:HA2 | 0.43 | 1.91 | 2 | 2 |
| 1:A:20:ASP:O | 1:A:47:ILE:HB | 0.43 | 2.14 | 3 | 2 |
| 1:A:70:CYS:O | 1:A:84:CYS:HA | 0.43 | 2.14 | 4 | 1 |
| 1:A:16:LEU:HA | 1:A:69:THR:O | 0.43 | 2.14 | 3 | 2 |
| 1:A:25:VAL:HG22 | 1:A:48:GLN:CD | 0.42 | 2.35 | 15 | 1 |
| 1:A:24:LYS:HA | 1:A:47:ILE:HA | 0.42 | 1.91 | 4 | 1 |
| 1:A:24:LYS:N | 1:A:24:LYS:HD2 | 0.42 | 2.29 | 4 | 1 |
| 1:A:56:ILE:HD12 | 1:A:56:ILE:N | 0.42 | 2.29 | 18 | 3 |
| 1:A:71:CYS:SG | 1:A:81:GLY:HA3 | 0.41 | 2.55 | 1 | 1 |
| 1:A:44:GLN:NE2 | 1:A:82:ILE:HG21 | 0.41 | 2.29 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:5:GLU:OE1 | 1:A:7:LYS:HG2 | 0.41 | 2.15 | 2 | 1 |
| 1:A:54:LEU:HD12 | 1:A:54:LEU:O | 0.41 | 2.16 | 14 | 1 |
| 1:A:75:GLU:O | 1:A:76:ASP:HB2 | 0.41 | 2.16 | 18 | 1 |
| 1:A:60:ILE:O | 1:A:63:GLU:HG3 | 0.40 | 2.17 | 12 | 1 |
| 1:A:18:CYS:HA | 1:A:67:THR:O | 0.40 | 2.16 | 18 | 1 |
| 1:A:52:ILE:HG23 | 1:A:53:PRO:HD2 | 0.40 | 1.93 | 2 | 2 |

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 | 74/90 (82%) | 68±2 (92±2%) | 5±2 (7±2%) | 1±1 (1±1%) | 17 | 67 |
| All | All | 1480/1800 (82%) | 1368 (92%) | 98 (7%) | 14 (1%) | 17 | 67 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 53 | PRO | 12 |
| 1 | A | 27 | LYS | 2 |

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 | 65/77 (84%) | 61±2 (94±2%) | 4±2 (6±2%) | 18 | 69 |
| All | All | 1300/1540 (84%) | 1220 (94%) | 80 (6%) | 18 | 69 |

All 22 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 58 | ILE | 20 |
| 1 | A | 7 | LYS | 13 |
| 1 | A | 24 | LYS | 10 |
| 1 | A | 48 | GLN | 7 |
| 1 | A | 61 | GLU | 6 |
| 1 | A | 84 | CYS | 3 |
| 1 | A | 74 | VAL | 3 |
| 1 | A | 12 | ASN | 3 |
| 1 | A | 29 | THR | 2 |
| 1 | A | 49 | CYS | 1 |
| 1 | A | 64 | CYS | 1 |
| 1 | A | 8 | THR | 1 |
| 1 | A | 19 | CYS | 1 |
| 1 | A | 27 | LYS | 1 |
| 1 | A | 23 | LYS | 1 |
| 1 | A | 75 | GLU | 1 |
| 1 | A | 69 | THR | 1 |
| 1 | A | 13 | THR | 1 |
| 1 | A | 76 | ASP | 1 |
| 1 | A | 51 | GLN | 1 |
| 1 | A | 5 | GLU | 1 |
| 1 | A | 72 | GLU | 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 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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 | 1013 |
| Number of shifts mapped to atoms | 1013 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 89 | -0.03 ± 0.09 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 79 | -0.03 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 86 | 0.12 ± 0.12 | None needed (< 0.5 ppm) |
| ^{15}N | 79 | -0.39 ± 0.25 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 838 atoms were assigned a chemical shift out of a possible 910. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 355/368 (96%) | 146/150 (97%) | 144/148 (97%) | 65/70 (93%) |
| Sidechain | 471/530 (89%) | 310/342 (91%) | 153/174 (88%) | 8/14 (57%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 12/12 (100%) | 6/6 (100%) | 5/5 (100%) | 1/1 (100%) |
| Overall | 838/910 (92%) | 462/498 (93%) | 302/327 (92%) | 74/85 (87%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1013 atoms were assigned a chemical shift out of a possible 1100. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 432/452 (96%) | 178/186 (96%) | 175/180 (97%) | 79/86 (92%) |
| Sidechain | 565/628 (90%) | 374/408 (92%) | 183/206 (89%) | 8/14 (57%) |
| Aromatic | 16/20 (80%) | 8/10 (80%) | 7/7 (100%) | 1/3 (33%) |
| Overall | 1013/1100 (92%) | 560/604 (93%) | 365/393 (93%) | 88/103 (85%) |

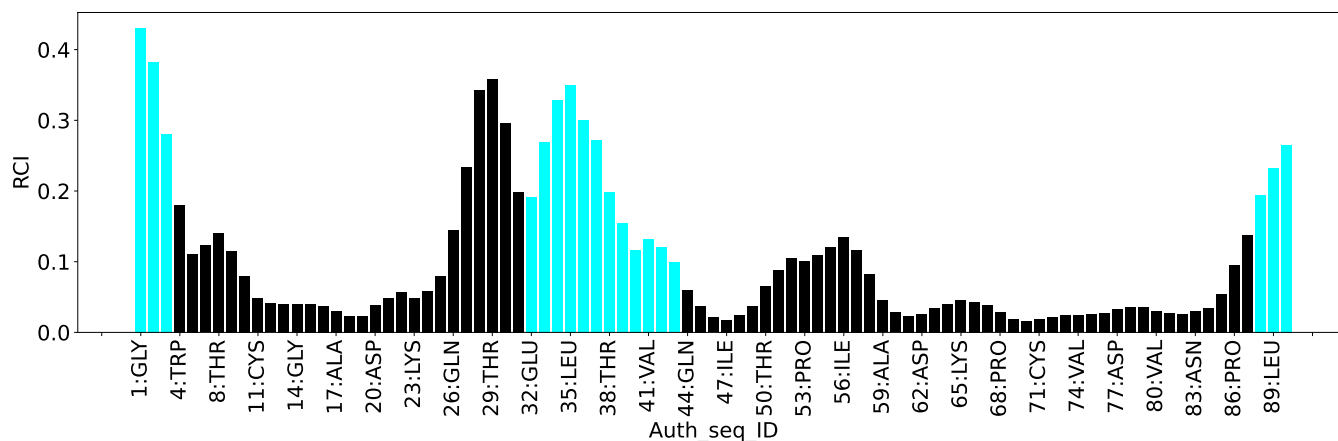
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 1328 |
| Intra-residue ($ i-j =0$) | 676 |
| Sequential ($ i-j =1$) | 309 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 71 |
| Long range ($ i-j \geq 5$) | 270 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 2 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 162 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 16.6 |
| Number of long range restraints per residue ¹ | 3.0 |

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) | 40.9 | 0.2 |
| 0.2-0.5 (Medium) | 76.8 | 0.5 |
| >0.5 (Large) | 66.3 | 3.41 |

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) | 10.7 | 7.81 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

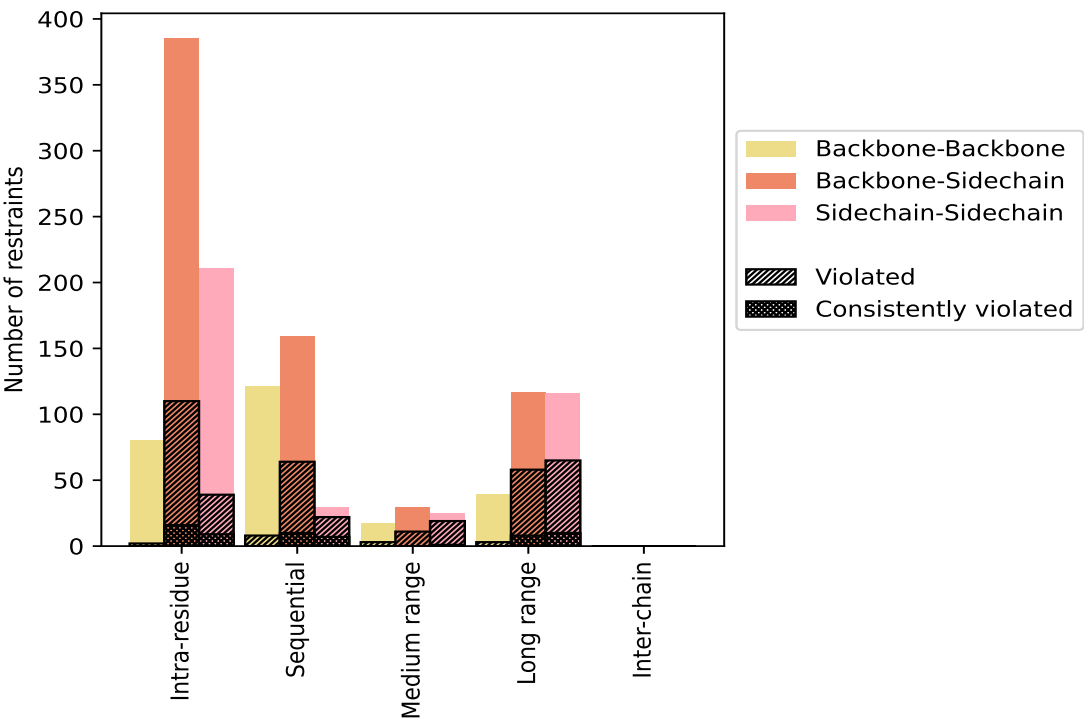
9.1 Summary of distance violations ⓘ

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

| Restraints type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 676 | 50.9 | 151 | 22.3 | 11.4 | 25 | 3.7 | 1.9 |
| Backbone-Backbone | 80 | 6.0 | 2 | 2.5 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 385 | 29.0 | 110 | 28.6 | 8.3 | 16 | 4.2 | 1.2 |
| Sidechain-Sidechain | 211 | 15.9 | 39 | 18.5 | 2.9 | 9 | 4.3 | 0.7 |
| Sequential ($i-j =1$) | 309 | 23.3 | 94 | 30.4 | 7.1 | 17 | 5.5 | 1.3 |
| Backbone-Backbone | 121 | 9.1 | 8 | 6.6 | 0.6 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 159 | 12.0 | 64 | 40.3 | 4.8 | 10 | 6.3 | 0.8 |
| Sidechain-Sidechain | 29 | 2.2 | 22 | 75.9 | 1.7 | 7 | 24.1 | 0.5 |
| Medium range ($i-j >1$ & $i-j <5$) | 71 | 5.3 | 33 | 46.5 | 2.5 | 1 | 1.4 | 0.1 |
| Backbone-Backbone | 17 | 1.3 | 3 | 17.6 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 29 | 2.2 | 11 | 37.9 | 0.8 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 25 | 1.9 | 19 | 76.0 | 1.4 | 1 | 4.0 | 0.1 |
| Long range ($i-j \geq 5$) | 270 | 20.3 | 126 | 46.7 | 9.5 | 18 | 6.7 | 1.4 |
| Backbone-Backbone | 39 | 2.9 | 3 | 7.7 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 115 | 8.7 | 58 | 50.4 | 4.4 | 8 | 7.0 | 0.6 |
| Sidechain-Sidechain | 116 | 8.7 | 65 | 56.0 | 4.9 | 10 | 8.6 | 0.8 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 2 | 0.2 | 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 | 1328 | 100.0 | 404 | 30.4 | 30.4 | 61 | 4.6 | 4.6 |
| Backbone-Backbone | 257 | 19.4 | 16 | 6.2 | 1.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 690 | 52.0 | 243 | 35.2 | 18.3 | 34 | 4.9 | 2.6 |
| Sidechain-Sidechain | 381 | 28.7 | 145 | 38.1 | 10.9 | 27 | 7.1 | 2.0 |

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 | 69 | 45 | 12 | 64 | 0 | 190 | 0.51 | 2.7 | 0.4 | 0.43 |
| 2 | 74 | 46 | 10 | 60 | 0 | 190 | 0.48 | 2.61 | 0.4 | 0.35 |
| 3 | 67 | 40 | 14 | 56 | 0 | 177 | 0.44 | 2.65 | 0.37 | 0.32 |
| 4 | 72 | 46 | 10 | 63 | 0 | 191 | 0.47 | 2.01 | 0.36 | 0.35 |
| 5 | 68 | 43 | 9 | 65 | 0 | 185 | 0.44 | 2.68 | 0.35 | 0.35 |
| 6 | 66 | 47 | 7 | 60 | 0 | 180 | 0.47 | 2.71 | 0.38 | 0.36 |
| 7 | 64 | 43 | 12 | 54 | 0 | 173 | 0.49 | 2.69 | 0.37 | 0.41 |
| 8 | 69 | 43 | 14 | 63 | 0 | 189 | 0.51 | 3.3 | 0.5 | 0.37 |
| 9 | 90 | 51 | 11 | 66 | 0 | 218 | 0.45 | 2.67 | 0.35 | 0.33 |
| 10 | 69 | 49 | 11 | 64 | 0 | 193 | 0.46 | 2.0 | 0.36 | 0.33 |

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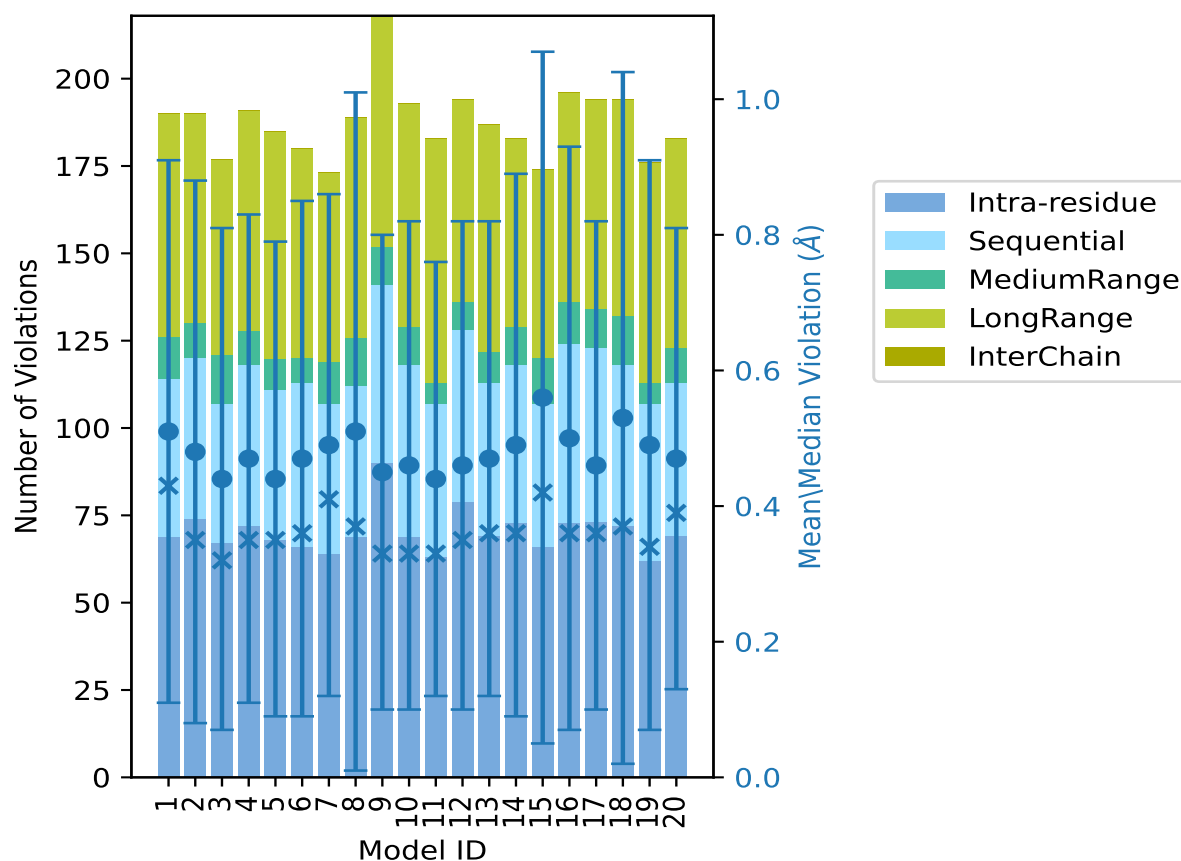
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 63 | 44 | 6 | 70 | 0 | 183 | 0.44 | 1.41 | 0.32 | 0.33 |
| 12 | 79 | 49 | 8 | 58 | 0 | 194 | 0.46 | 2.67 | 0.36 | 0.35 |
| 13 | 69 | 44 | 9 | 65 | 0 | 187 | 0.47 | 2.45 | 0.35 | 0.36 |
| 14 | 73 | 45 | 11 | 54 | 0 | 183 | 0.49 | 2.64 | 0.4 | 0.36 |
| 15 | 66 | 41 | 13 | 54 | 0 | 174 | 0.56 | 3.36 | 0.51 | 0.42 |
| 16 | 73 | 51 | 12 | 60 | 0 | 196 | 0.5 | 2.96 | 0.43 | 0.36 |
| 17 | 73 | 50 | 11 | 60 | 0 | 194 | 0.46 | 2.75 | 0.36 | 0.36 |
| 18 | 72 | 46 | 14 | 62 | 0 | 194 | 0.53 | 3.41 | 0.51 | 0.37 |
| 19 | 62 | 45 | 6 | 63 | 0 | 176 | 0.49 | 2.68 | 0.42 | 0.34 |
| 20 | 69 | 44 | 10 | 60 | 0 | 183 | 0.47 | 2.03 | 0.34 | 0.39 |

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

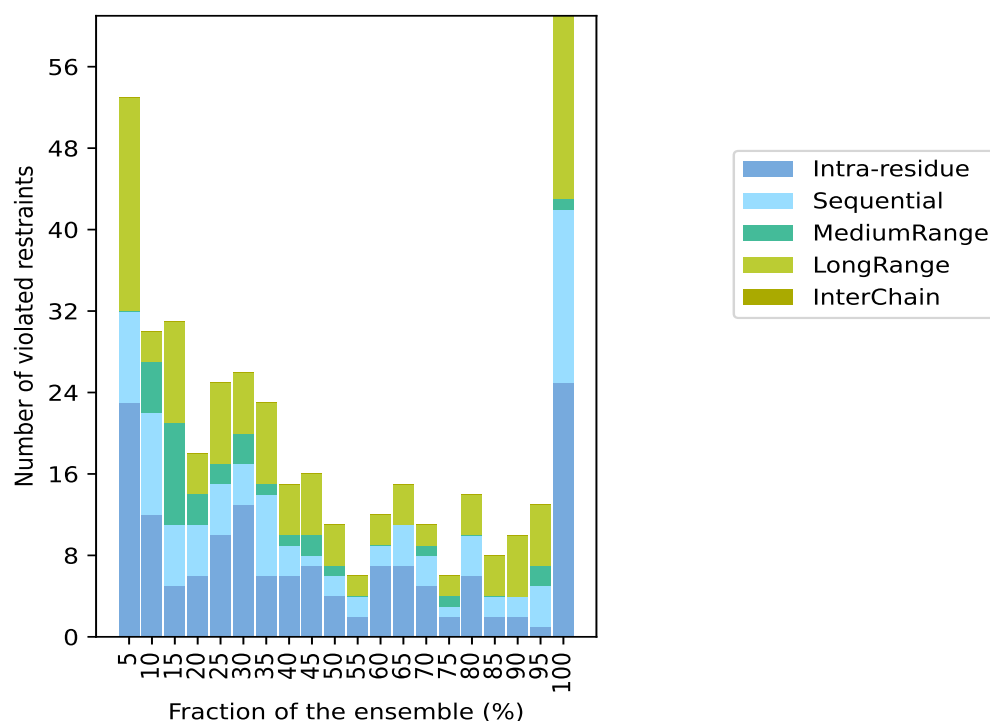
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 922(IR:525, SQ:215, MR:38, LR:144, IC:0) restraints are not 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 | % |
| 23 | 9 | 0 | 21 | 0 | 53 | 1 | 5.0 |
| 12 | 10 | 5 | 3 | 0 | 30 | 2 | 10.0 |
| 5 | 6 | 10 | 10 | 0 | 31 | 3 | 15.0 |
| 6 | 5 | 3 | 4 | 0 | 18 | 4 | 20.0 |
| 10 | 5 | 2 | 8 | 0 | 25 | 5 | 25.0 |
| 13 | 4 | 3 | 6 | 0 | 26 | 6 | 30.0 |
| 6 | 8 | 1 | 8 | 0 | 23 | 7 | 35.0 |
| 6 | 3 | 1 | 5 | 0 | 15 | 8 | 40.0 |
| 7 | 1 | 2 | 6 | 0 | 16 | 9 | 45.0 |
| 4 | 2 | 1 | 4 | 0 | 11 | 10 | 50.0 |
| 2 | 2 | 0 | 2 | 0 | 6 | 11 | 55.0 |
| 7 | 2 | 0 | 3 | 0 | 12 | 12 | 60.0 |
| 7 | 4 | 0 | 4 | 0 | 15 | 13 | 65.0 |
| 5 | 3 | 1 | 2 | 0 | 11 | 14 | 70.0 |
| 2 | 1 | 1 | 2 | 0 | 6 | 15 | 75.0 |
| 6 | 4 | 0 | 4 | 0 | 14 | 16 | 80.0 |
| 2 | 2 | 0 | 4 | 0 | 8 | 17 | 85.0 |
| 2 | 2 | 0 | 6 | 0 | 10 | 18 | 90.0 |
| 1 | 4 | 2 | 6 | 0 | 13 | 19 | 95.0 |
| 25 | 17 | 1 | 18 | 0 | 61 | 20 | 100.0 |

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

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

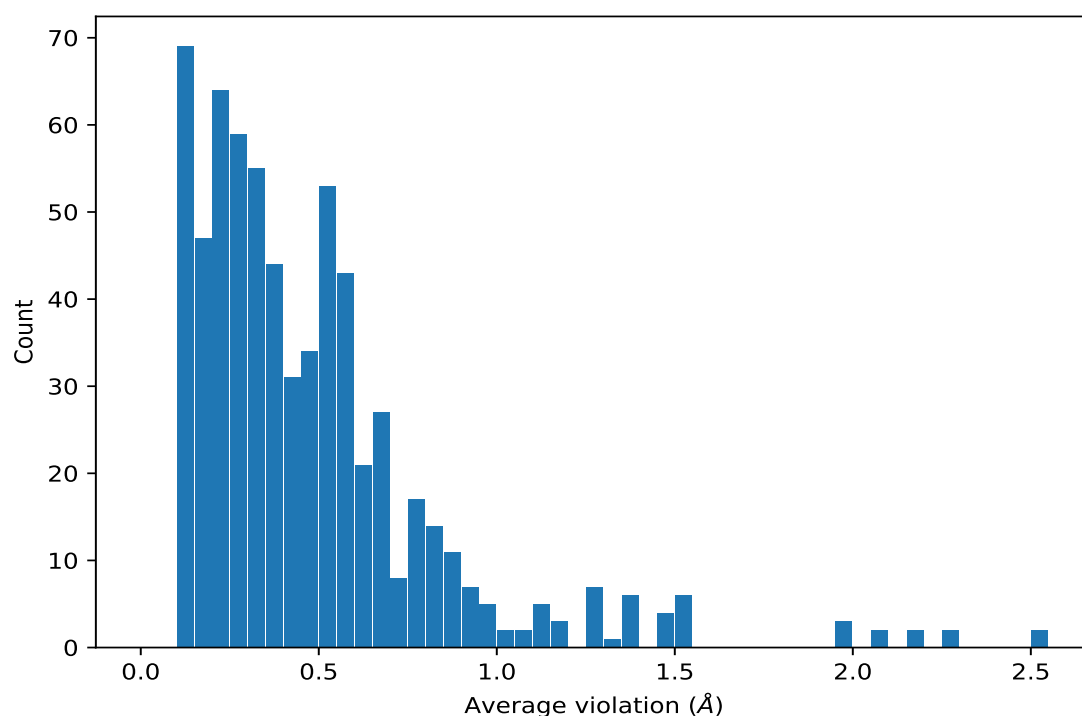
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 20 | 1.96 | 1.1 | 2.67 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 20 | 1.96 | 1.1 | 2.67 |
| (2,459) | 1:45:A:VAL:HG13 | 1:44:A:GLN:HA | 20 | 1.96 | 1.1 | 2.67 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 20 | 1.39 | 0.04 | 1.4 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 20 | 1.39 | 0.04 | 1.4 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 20 | 1.39 | 0.04 | 1.4 |
| (2,112) | 1:67:A:THR:HG21 | 1:68:A:PRO:HG3 | 20 | 1.27 | 0.12 | 1.21 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 20 | 1.27 | 0.12 | 1.21 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 20 | 1.27 | 0.12 | 1.21 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 20 | 1.11 | 0.19 | 1.12 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 20 | 0.94 | 0.33 | 1.02 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 20 | 0.92 | 0.35 | 1.12 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 20 | 0.92 | 0.35 | 1.12 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 20 | 0.92 | 0.35 | 1.12 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 20 | 0.89 | 0.01 | 0.89 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 20 | 0.87 | 0.51 | 1.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 20 | 0.87 | 0.51 | 1.23 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD23 | 20 | 0.87 | 0.51 | 1.23 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 20 | 0.83 | 0.17 | 0.84 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 20 | 0.83 | 0.17 | 0.84 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 20 | 0.83 | 0.17 | 0.84 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 20 | 0.82 | 0.19 | 0.9 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD13 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD12 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD13 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD11 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD12 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD12 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD11 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD13 | 20 | 0.75 | 0.04 | 0.74 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD11 | 20 | 0.75 | 0.04 | 0.74 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 20 | 0.73 | 0.44 | 0.64 |
| (2,1167) | 1:47:A:ILE:HG22 | 1:20:A:ASP:H | 20 | 0.68 | 0.04 | 0.68 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 20 | 0.68 | 0.04 | 0.68 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 20 | 0.68 | 0.04 | 0.68 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 20 | 0.68 | 1.13 | 0.21 |
| (2,228) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA3 | 20 | 0.68 | 1.13 | 0.21 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 20 | 0.68 | 1.13 | 0.21 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 20 | 0.65 | 0.07 | 0.64 |
| (2,892) | 1:69:A:THR:HG22 | 1:19:A:CYS:HA | 20 | 0.65 | 0.07 | 0.64 |
| (2,892) | 1:69:A:THR:HG23 | 1:19:A:CYS:HA | 20 | 0.65 | 0.07 | 0.64 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 20 | 0.65 | 0.25 | 0.74 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 20 | 0.63 | 0.28 | 0.72 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 20 | 0.63 | 0.28 | 0.72 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB2 | 20 | 0.63 | 0.28 | 0.72 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 20 | 0.62 | 0.12 | 0.66 |
| (2,1253) | 1:16:A:LEU:HD13 | 1:4:A:TRP:HE1 | 20 | 0.62 | 0.12 | 0.66 |
| (2,1253) | 1:16:A:LEU:HD12 | 1:4:A:TRP:HE1 | 20 | 0.62 | 0.12 | 0.66 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 20 | 0.62 | 0.03 | 0.63 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 20 | 0.62 | 0.03 | 0.63 |
| (2,62) | 1:50:A:THR:HG22 | 1:50:A:THR:HA | 20 | 0.62 | 0.03 | 0.63 |
| (2,40) | 1:46:A:ALA:HB1 | 1:45:A:VAL:HA | 20 | 0.62 | 0.05 | 0.62 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 20 | 0.62 | 0.05 | 0.62 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 20 | 0.62 | 0.05 | 0.62 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 20 | 0.57 | 0.04 | 0.56 |
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 20 | 0.57 | 0.04 | 0.56 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 20 | 0.57 | 0.04 | 0.56 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 20 | 0.57 | 0.04 | 0.57 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 20 | 0.57 | 0.04 | 0.57 |
| (2,1086) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 20 | 0.57 | 0.04 | 0.57 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 20 | 0.56 | 0.02 | 0.56 |
| (2,292) | 1:16:A:LEU:HD13 | 1:16:A:LEU:HB3 | 20 | 0.56 | 0.02 | 0.56 |
| (2,292) | 1:16:A:LEU:HD12 | 1:16:A:LEU:HB3 | 20 | 0.56 | 0.02 | 0.56 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 20 | 0.56 | 0.1 | 0.56 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 20 | 0.56 | 0.1 | 0.56 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 20 | 0.56 | 0.1 | 0.56 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG22 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG23 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB2 | 1:25:A:VAL:HG22 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB2 | 1:25:A:VAL:HG21 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG22 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG21 | 20 | 0.55 | 0.08 | 0.56 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG21 | 20 | 0.55 | 0.08 | 0.56 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG23 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG23 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG22 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG23 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG21 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG22 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG21 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG21 | 20 | 0.54 | 0.05 | 0.54 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG22 | 20 | 0.54 | 0.05 | 0.54 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 20 | 0.53 | 0.24 | 0.48 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 20 | 0.53 | 0.24 | 0.48 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 20 | 0.53 | 0.24 | 0.48 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 20 | 0.53 | 0.08 | 0.52 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 20 | 0.53 | 0.18 | 0.64 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD11 | 20 | 0.52 | 0.01 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 20 | 0.52 | 0.01 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD12 | 20 | 0.52 | 0.01 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 20 | 0.52 | 0.02 | 0.52 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 20 | 0.51 | 0.07 | 0.53 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG22 | 20 | 0.51 | 0.07 | 0.53 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 20 | 0.51 | 0.07 | 0.53 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 20 | 0.5 | 0.04 | 0.5 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 20 | 0.5 | 0.04 | 0.5 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 20 | 0.5 | 0.04 | 0.5 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 20 | 0.5 | 0.1 | 0.52 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 20 | 0.5 | 0.1 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,24) | 1:41:A:VAL:HG11 | 1:42:A:LEU:H | 20 | 0.5 | 0.1 | 0.52 |
| (1,24) | 1:41:A:VAL:HG21 | 1:42:A:LEU:H | 20 | 0.5 | 0.1 | 0.52 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 20 | 0.48 | 0.08 | 0.5 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 20 | 0.48 | 0.08 | 0.5 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 20 | 0.48 | 0.08 | 0.5 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 20 | 0.47 | 0.04 | 0.48 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 20 | 0.47 | 0.04 | 0.48 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 20 | 0.47 | 0.04 | 0.48 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 20 | 0.45 | 0.04 | 0.46 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 20 | 0.45 | 0.04 | 0.46 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD12 | 20 | 0.45 | 0.04 | 0.46 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 20 | 0.42 | 0.04 | 0.42 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 20 | 0.42 | 0.04 | 0.42 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 20 | 0.42 | 0.04 | 0.42 |
| (2,1143) | 1:25:A:VAL:HG23 | 1:24:A:LYS:H | 20 | 0.41 | 0.12 | 0.42 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 20 | 0.41 | 0.12 | 0.42 |
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 20 | 0.41 | 0.12 | 0.42 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 20 | 0.38 | 0.17 | 0.42 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 20 | 0.38 | 0.17 | 0.42 |
| (2,815) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB3 | 20 | 0.38 | 0.17 | 0.42 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 20 | 0.38 | 0.2 | 0.4 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 20 | 0.38 | 0.06 | 0.38 |
| (2,1151) | 1:80:A:VAL:HG23 | 1:81:A:GLY:H | 20 | 0.38 | 0.06 | 0.38 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 20 | 0.38 | 0.06 | 0.38 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 20 | 0.38 | 0.11 | 0.42 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 20 | 0.38 | 0.11 | 0.42 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD11 | 20 | 0.38 | 0.11 | 0.42 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 20 | 0.36 | 0.05 | 0.36 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 20 | 0.36 | 0.05 | 0.36 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 20 | 0.36 | 0.05 | 0.36 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 20 | 0.35 | 0.05 | 0.35 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 20 | 0.35 | 0.05 | 0.35 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 20 | 0.35 | 0.05 | 0.35 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 20 | 0.33 | 0.01 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD12 | 20 | 0.33 | 0.01 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 20 | 0.33 | 0.01 | 0.33 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 20 | 0.31 | 0.0 | 0.31 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 20 | 0.3 | 0.04 | 0.31 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 20 | 0.3 | 0.04 | 0.31 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB2 | 20 | 0.3 | 0.04 | 0.31 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 20 | 0.28 | 0.0 | 0.28 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG21 | 20 | 0.27 | 0.05 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 20 | 0.27 | 0.05 | 0.29 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 20 | 0.27 | 0.05 | 0.29 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 20 | 0.26 | 0.01 | 0.27 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD23 | 20 | 0.26 | 0.03 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 20 | 0.26 | 0.03 | 0.28 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD22 | 20 | 0.26 | 0.03 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD23 | 20 | 0.26 | 0.03 | 0.28 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD21 | 20 | 0.26 | 0.03 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD21 | 20 | 0.26 | 0.03 | 0.28 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 20 | 0.25 | 0.05 | 0.23 |
| (2,603) | 1:16:A:LEU:HD11 | 1:70:A:CYS:HA | 20 | 0.25 | 0.05 | 0.23 |
| (2,603) | 1:16:A:LEU:HD13 | 1:70:A:CYS:HA | 20 | 0.25 | 0.05 | 0.23 |
| (2,599) | 1:47:A:ILE:HG22 | 1:21:A:THR:HB | 20 | 0.24 | 0.04 | 0.24 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 20 | 0.24 | 0.04 | 0.24 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 20 | 0.24 | 0.04 | 0.24 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 20 | 0.24 | 0.03 | 0.24 |
| (2,99) | 1:58:A:ILE:HG22 | 1:58:A:ILE:HA | 20 | 0.24 | 0.03 | 0.24 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 20 | 0.24 | 0.03 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 20 | 0.23 | 0.02 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 20 | 0.23 | 0.02 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG22 | 20 | 0.23 | 0.02 | 0.24 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 20 | 0.23 | 0.06 | 0.26 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 20 | 0.21 | 0.02 | 0.21 |
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 20 | 0.21 | 0.02 | 0.21 |
| (2,885) | 1:47:A:ILE:HD13 | 1:47:A:ILE:HA | 20 | 0.21 | 0.02 | 0.21 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 20 | 0.18 | 0.03 | 0.17 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD11 | 20 | 0.18 | 0.03 | 0.17 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD13 | 20 | 0.18 | 0.03 | 0.17 |
| (2,422) | 1:79:A:LEU:HD12 | 1:79:A:LEU:HG | 20 | 0.13 | 0.01 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 20 | 0.13 | 0.01 | 0.14 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 20 | 0.13 | 0.01 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 20 | 0.13 | 0.01 | 0.13 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 19 | 1.54 | 0.85 | 1.07 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 19 | 1.54 | 0.85 | 1.07 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 19 | 1.54 | 0.85 | 1.07 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 19 | 1.35 | 0.42 | 1.28 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 19 | 1.35 | 0.42 | 1.28 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 19 | 1.35 | 0.42 | 1.28 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 19 | 1.17 | 0.49 | 1.19 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 19 | 1.17 | 0.49 | 1.19 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG21 | 19 | 1.17 | 0.49 | 1.19 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 19 | 1.11 | 0.09 | 1.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,682) | 1:17:A:ALA:HB2 | 1:18:A:CYS:HB3 | 19 | 1.11 | 0.09 | 1.12 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 19 | 1.11 | 0.09 | 1.12 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG22 | 19 | 0.77 | 0.23 | 0.76 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG23 | 19 | 0.77 | 0.23 | 0.76 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 19 | 0.77 | 0.23 | 0.76 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 19 | 0.73 | 0.28 | 0.87 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 19 | 0.59 | 0.11 | 0.61 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 19 | 0.45 | 0.14 | 0.47 |
| (2,323) | 1:69:A:THR:HG21 | 1:86:A:PRO:HD2 | 19 | 0.45 | 0.14 | 0.47 |
| (2,323) | 1:69:A:THR:HG22 | 1:86:A:PRO:HD2 | 19 | 0.45 | 0.14 | 0.47 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 19 | 0.41 | 0.18 | 0.5 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 19 | 0.38 | 0.1 | 0.38 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 19 | 0.26 | 0.11 | 0.23 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 19 | 0.24 | 0.06 | 0.26 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 19 | 0.24 | 0.06 | 0.26 |
| (2,856) | 1:90:A:ILE:HD11 | 1:88:A:PRO:HG3 | 19 | 0.24 | 0.06 | 0.26 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 19 | 0.17 | 0.03 | 0.18 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 18 | 1.28 | 0.37 | 1.26 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG23 | 18 | 0.99 | 0.28 | 1.11 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 18 | 0.99 | 0.28 | 1.11 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG21 | 18 | 0.99 | 0.28 | 1.11 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 18 | 0.58 | 0.04 | 0.58 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 18 | 0.58 | 0.04 | 0.58 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD12 | 18 | 0.58 | 0.04 | 0.58 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 18 | 0.38 | 0.17 | 0.4 |
| (2,180) | 1:69:A:THR:HG21 | 1:86:A:PRO:HB2 | 18 | 0.38 | 0.17 | 0.4 |
| (2,180) | 1:69:A:THR:HG22 | 1:86:A:PRO:HB2 | 18 | 0.38 | 0.17 | 0.4 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 18 | 0.33 | 0.03 | 0.33 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 18 | 0.33 | 0.03 | 0.33 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD11 | 18 | 0.33 | 0.03 | 0.33 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 18 | 0.31 | 0.16 | 0.27 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 18 | 0.29 | 0.04 | 0.28 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 18 | 0.28 | 0.1 | 0.28 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 18 | 0.28 | 0.1 | 0.28 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 18 | 0.28 | 0.1 | 0.28 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 18 | 0.25 | 0.06 | 0.28 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 18 | 0.15 | 0.02 | 0.15 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 17 | 0.93 | 0.05 | 0.94 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 17 | 0.72 | 0.43 | 1.05 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 17 | 0.45 | 0.2 | 0.36 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 17 | 0.31 | 0.07 | 0.31 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 17 | 0.31 | 0.07 | 0.31 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,298) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HB3 | 17 | 0.31 | 0.07 | 0.31 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 17 | 0.29 | 0.05 | 0.28 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG23 | 17 | 0.27 | 0.06 | 0.3 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG22 | 17 | 0.27 | 0.06 | 0.3 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 17 | 0.27 | 0.06 | 0.3 |
| (2,923) | 1:21:A:THR:HG22 | 1:67:A:THR:HB | 17 | 0.17 | 0.03 | 0.16 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 17 | 0.17 | 0.03 | 0.16 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 17 | 0.17 | 0.03 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 17 | 0.16 | 0.02 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG22 | 17 | 0.16 | 0.02 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG21 | 17 | 0.16 | 0.02 | 0.16 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 16 | 0.83 | 0.36 | 0.82 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 16 | 0.52 | 0.17 | 0.6 |
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 16 | 0.5 | 0.17 | 0.49 |
| (2,1210) | 1:46:A:ALA:HB2 | 1:26:A:GLN:H | 16 | 0.5 | 0.17 | 0.49 |
| (2,1210) | 1:46:A:ALA:HB3 | 1:26:A:GLN:H | 16 | 0.5 | 0.17 | 0.49 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 16 | 0.45 | 0.26 | 0.3 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 16 | 0.4 | 0.1 | 0.43 |
| (2,600) | 1:47:A:ILE:HD11 | 1:21:A:THR:HB | 16 | 0.4 | 0.1 | 0.43 |
| (2,600) | 1:47:A:ILE:HD13 | 1:21:A:THR:HB | 16 | 0.4 | 0.1 | 0.43 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 16 | 0.35 | 0.42 | 0.15 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 16 | 0.3 | 0.07 | 0.31 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 16 | 0.3 | 0.07 | 0.31 |
| (2,109) | 1:13:A:THR:HG23 | 1:12:A:ASN:HB2 | 16 | 0.3 | 0.07 | 0.31 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 16 | 0.25 | 0.01 | 0.25 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 16 | 0.22 | 0.08 | 0.2 |
| (2,1068) | 1:47:A:ILE:HG22 | 1:21:A:THR:H | 16 | 0.22 | 0.07 | 0.22 |
| (2,1068) | 1:47:A:ILE:HG21 | 1:21:A:THR:H | 16 | 0.22 | 0.07 | 0.22 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 16 | 0.22 | 0.07 | 0.22 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 16 | 0.13 | 0.02 | 0.13 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 16 | 0.13 | 0.04 | 0.11 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 16 | 0.12 | 0.01 | 0.12 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 16 | 0.12 | 0.04 | 0.11 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 15 | 0.74 | 0.17 | 0.81 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 15 | 0.69 | 0.02 | 0.69 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 15 | 0.69 | 0.34 | 0.57 |
| (2,1255) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE21 | 15 | 0.69 | 0.28 | 0.61 |
| (2,1255) | 1:82:A:ILE:HD11 | 1:44:A:GLN:HE21 | 15 | 0.69 | 0.28 | 0.61 |
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 15 | 0.69 | 0.28 | 0.61 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 15 | 0.5 | 0.06 | 0.52 |
| (2,502) | 1:58:A:ILE:HG23 | 1:63:A:GLU:HG3 | 15 | 0.5 | 0.06 | 0.52 |
| (2,502) | 1:58:A:ILE:HG21 | 1:63:A:GLU:HG3 | 15 | 0.5 | 0.06 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 15 | 0.25 | 0.01 | 0.24 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 14 | 1.26 | 0.03 | 1.25 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 14 | 1.26 | 0.03 | 1.25 |
| (2,1225) | 1:45:A:VAL:HG11 | 1:45:A:VAL:H | 14 | 1.26 | 0.03 | 1.25 |
| (2,24) | 1:60:A:ILE:HD13 | 1:60:A:ILE:HG21 | 14 | 0.86 | 0.05 | 0.86 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG21 | 14 | 0.86 | 0.05 | 0.86 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG22 | 14 | 0.86 | 0.05 | 0.86 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG23 | 14 | 0.86 | 0.05 | 0.86 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG22 | 14 | 0.86 | 0.05 | 0.86 |
| (2,24) | 1:60:A:ILE:HD13 | 1:60:A:ILE:HG22 | 14 | 0.86 | 0.05 | 0.86 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG23 | 14 | 0.86 | 0.05 | 0.86 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 14 | 0.84 | 0.07 | 0.85 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 14 | 0.73 | 0.42 | 0.68 |
| (2,940) | 1:79:A:LEU:HD23 | 1:49:A:CYS:H | 14 | 0.73 | 0.42 | 0.68 |
| (2,940) | 1:79:A:LEU:HD21 | 1:49:A:CYS:H | 14 | 0.73 | 0.42 | 0.68 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 14 | 0.66 | 0.27 | 0.76 |
| (2,1158) | 1:45:A:VAL:HG22 | 1:46:A:ALA:H | 14 | 0.64 | 0.1 | 0.64 |
| (2,1158) | 1:45:A:VAL:HG23 | 1:46:A:ALA:H | 14 | 0.64 | 0.1 | 0.64 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 14 | 0.64 | 0.1 | 0.64 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 14 | 0.52 | 0.41 | 0.32 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD11 | 14 | 0.52 | 0.41 | 0.32 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD12 | 14 | 0.52 | 0.41 | 0.32 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 14 | 0.37 | 0.11 | 0.42 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 14 | 0.16 | 0.05 | 0.14 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 14 | 0.14 | 0.02 | 0.14 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 14 | 0.13 | 0.02 | 0.12 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 13 | 0.84 | 0.44 | 0.78 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 13 | 0.79 | 0.27 | 0.79 |
| (2,863) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB2 | 13 | 0.58 | 0.19 | 0.54 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 13 | 0.58 | 0.19 | 0.54 |
| (2,863) | 1:41:A:VAL:HG13 | 1:40:A:ASP:HB2 | 13 | 0.58 | 0.19 | 0.54 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 13 | 0.51 | 0.42 | 0.42 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 13 | 0.32 | 0.07 | 0.34 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD13 | 13 | 0.32 | 0.07 | 0.34 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD11 | 13 | 0.32 | 0.07 | 0.34 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 13 | 0.31 | 0.01 | 0.31 |
| (2,1290) | 1:60:A:ILE:HD13 | 1:19:A:CYS:H | 13 | 0.3 | 0.11 | 0.29 |
| (2,1290) | 1:60:A:ILE:HD12 | 1:19:A:CYS:H | 13 | 0.3 | 0.11 | 0.29 |
| (2,1290) | 1:60:A:ILE:HD11 | 1:19:A:CYS:H | 13 | 0.3 | 0.11 | 0.29 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 13 | 0.27 | 0.01 | 0.27 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD11 | 13 | 0.23 | 0.08 | 0.22 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD13 | 13 | 0.23 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD12 | 13 | 0.23 | 0.08 | 0.22 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 13 | 0.22 | 0.02 | 0.22 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG22 | 13 | 0.2 | 0.08 | 0.18 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG21 | 13 | 0.2 | 0.08 | 0.18 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG23 | 13 | 0.2 | 0.08 | 0.18 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG23 | 13 | 0.19 | 0.04 | 0.2 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG21 | 13 | 0.19 | 0.04 | 0.2 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG22 | 13 | 0.19 | 0.04 | 0.2 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 13 | 0.14 | 0.02 | 0.13 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 13 | 0.13 | 0.01 | 0.14 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 13 | 0.11 | 0.01 | 0.11 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 12 | 1.03 | 0.24 | 1.12 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 12 | 0.66 | 0.03 | 0.66 |
| (2,205) | 1:74:A:VAL:HG23 | 1:15:A:LYS:HE3 | 12 | 0.56 | 0.31 | 0.62 |
| (2,205) | 1:74:A:VAL:HG21 | 1:15:A:LYS:HE3 | 12 | 0.56 | 0.31 | 0.62 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 12 | 0.56 | 0.31 | 0.62 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 12 | 0.55 | 0.03 | 0.56 |
| (2,225) | 1:54:A:LEU:HD23 | 1:54:A:LEU:HA | 12 | 0.52 | 0.02 | 0.53 |
| (2,225) | 1:54:A:LEU:HD21 | 1:54:A:LEU:HA | 12 | 0.52 | 0.02 | 0.53 |
| (2,225) | 1:54:A:LEU:HD22 | 1:54:A:LEU:HA | 12 | 0.52 | 0.02 | 0.53 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 12 | 0.38 | 0.06 | 0.37 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 12 | 0.35 | 0.16 | 0.37 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 12 | 0.32 | 0.03 | 0.33 |
| (1,14) | 1:42:A:LEU:HG | 1:42:A:LEU:HA | 12 | 0.32 | 0.03 | 0.33 |
| (2,1032) | 1:87:A:ILE:HG22 | 1:10:A:SER:H | 12 | 0.3 | 0.07 | 0.32 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 12 | 0.3 | 0.07 | 0.32 |
| (2,1032) | 1:87:A:ILE:HG23 | 1:10:A:SER:H | 12 | 0.3 | 0.07 | 0.32 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 12 | 0.29 | 0.12 | 0.24 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 12 | 0.18 | 0.13 | 0.13 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG21 | 12 | 0.14 | 0.03 | 0.12 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG23 | 12 | 0.14 | 0.03 | 0.12 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG22 | 12 | 0.14 | 0.03 | 0.12 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD21 | 11 | 0.6 | 0.05 | 0.61 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 11 | 0.6 | 0.05 | 0.61 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD22 | 11 | 0.6 | 0.05 | 0.61 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 11 | 0.5 | 0.43 | 0.19 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 11 | 0.42 | 0.26 | 0.3 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 11 | 0.32 | 0.21 | 0.18 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 11 | 0.17 | 0.04 | 0.18 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 11 | 0.13 | 0.02 | 0.12 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD13 | 10 | 1.49 | 0.87 | 2.0 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD11 | 10 | 1.49 | 0.87 | 2.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD12 | 10 | 1.49 | 0.87 | 2.0 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 10 | 0.82 | 0.71 | 0.76 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 10 | 0.49 | 0.04 | 0.5 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 10 | 0.46 | 0.03 | 0.46 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 10 | 0.41 | 0.04 | 0.4 |
| (2,711) | 1:25:A:VAL:HG21 | 1:48:A:GLN:HG2 | 10 | 0.35 | 0.07 | 0.32 |
| (2,711) | 1:25:A:VAL:HG22 | 1:48:A:GLN:HG2 | 10 | 0.35 | 0.07 | 0.32 |
| (2,711) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HG2 | 10 | 0.35 | 0.07 | 0.32 |
| (2,541) | 1:87:A:ILE:HG23 | 1:10:A:SER:HA | 10 | 0.33 | 0.11 | 0.36 |
| (2,541) | 1:87:A:ILE:HG22 | 1:10:A:SER:HA | 10 | 0.33 | 0.11 | 0.36 |
| (2,541) | 1:87:A:ILE:HG21 | 1:10:A:SER:HA | 10 | 0.33 | 0.11 | 0.36 |
| (2,1078) | 1:29:A:THR:HG22 | 1:29:A:THR:H | 10 | 0.26 | 0.04 | 0.27 |
| (2,1078) | 1:29:A:THR:HG23 | 1:29:A:THR:H | 10 | 0.26 | 0.04 | 0.27 |
| (2,1078) | 1:29:A:THR:HG21 | 1:29:A:THR:H | 10 | 0.26 | 0.04 | 0.27 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 10 | 0.22 | 0.01 | 0.22 |
| (2,1216) | 1:46:A:ALA:HB2 | 1:83:A:ASN:H | 10 | 0.2 | 0.08 | 0.17 |
| (2,1216) | 1:46:A:ALA:HB1 | 1:83:A:ASN:H | 10 | 0.2 | 0.08 | 0.17 |
| (2,1216) | 1:46:A:ALA:HB3 | 1:83:A:ASN:H | 10 | 0.2 | 0.08 | 0.17 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 10 | 0.17 | 0.05 | 0.15 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 9 | 0.82 | 0.54 | 0.79 |
| (2,543) | 1:79:A:LEU:HD21 | 1:50:A:THR:HA | 9 | 0.82 | 0.54 | 0.79 |
| (2,543) | 1:79:A:LEU:HD23 | 1:50:A:THR:HA | 9 | 0.82 | 0.54 | 0.79 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG23 | 9 | 0.79 | 0.4 | 0.85 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG21 | 9 | 0.79 | 0.4 | 0.85 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG22 | 9 | 0.79 | 0.4 | 0.85 |
| (2,428) | 1:59:A:ALA:HB1 | 1:62:A:ASP:HB3 | 9 | 0.67 | 0.33 | 0.66 |
| (2,428) | 1:59:A:ALA:HB3 | 1:62:A:ASP:HB3 | 9 | 0.67 | 0.33 | 0.66 |
| (2,428) | 1:59:A:ALA:HB2 | 1:62:A:ASP:HB3 | 9 | 0.67 | 0.33 | 0.66 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 9 | 0.61 | 0.21 | 0.57 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG22 | 9 | 0.55 | 0.07 | 0.52 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG21 | 9 | 0.55 | 0.07 | 0.52 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG23 | 9 | 0.55 | 0.07 | 0.52 |
| (1,30) | 1:35:A:LEU:HD22 | 1:36:A:LEU:H | 9 | 0.47 | 0.05 | 0.47 |
| (1,30) | 1:35:A:LEU:HD23 | 1:36:A:LEU:H | 9 | 0.47 | 0.05 | 0.47 |
| (1,30) | 1:35:A:LEU:HD21 | 1:36:A:LEU:H | 9 | 0.47 | 0.05 | 0.47 |
| (1,30) | 1:35:A:LEU:HD11 | 1:36:A:LEU:H | 9 | 0.47 | 0.05 | 0.47 |
| (1,30) | 1:35:A:LEU:HD12 | 1:36:A:LEU:H | 9 | 0.47 | 0.05 | 0.47 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 9 | 0.45 | 0.24 | 0.47 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 9 | 0.44 | 0.09 | 0.43 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 9 | 0.4 | 0.02 | 0.41 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG23 | 9 | 0.38 | 0.11 | 0.39 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG21 | 9 | 0.38 | 0.11 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG22 | 9 | 0.38 | 0.11 | 0.39 |
| (2,260) | 1:69:A:THR:HG22 | 1:19:A:CYS:HB3 | 9 | 0.22 | 0.02 | 0.23 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 9 | 0.22 | 0.02 | 0.23 |
| (2,260) | 1:69:A:THR:HG23 | 1:19:A:CYS:HB3 | 9 | 0.22 | 0.02 | 0.23 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 9 | 0.22 | 0.05 | 0.21 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 9 | 0.22 | 0.07 | 0.21 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 9 | 0.14 | 0.04 | 0.12 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 9 | 0.12 | 0.01 | 0.12 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 9 | 0.11 | 0.0 | 0.11 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 8 | 1.13 | 0.09 | 1.12 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 8 | 0.52 | 0.04 | 0.5 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 8 | 0.44 | 0.01 | 0.44 |
| (2,997) | 1:60:A:ILE:HD12 | 1:69:A:THR:H | 8 | 0.41 | 0.09 | 0.44 |
| (2,997) | 1:60:A:ILE:HD13 | 1:69:A:THR:H | 8 | 0.41 | 0.09 | 0.44 |
| (2,997) | 1:60:A:ILE:HD11 | 1:69:A:THR:H | 8 | 0.41 | 0.09 | 0.44 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 8 | 0.37 | 0.02 | 0.38 |
| (2,630) | 1:52:A:ILE:HD12 | 1:64:A:CYS:HB3 | 8 | 0.34 | 0.22 | 0.24 |
| (2,630) | 1:52:A:ILE:HD11 | 1:64:A:CYS:HB3 | 8 | 0.34 | 0.22 | 0.24 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 8 | 0.34 | 0.15 | 0.29 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 8 | 0.33 | 0.13 | 0.32 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 8 | 0.33 | 0.09 | 0.32 |
| (2,790) | 1:60:A:ILE:HD12 | 1:68:A:PRO:HA | 8 | 0.32 | 0.12 | 0.34 |
| (2,790) | 1:60:A:ILE:HD13 | 1:68:A:PRO:HA | 8 | 0.32 | 0.12 | 0.34 |
| (2,790) | 1:60:A:ILE:HD11 | 1:68:A:PRO:HA | 8 | 0.32 | 0.12 | 0.34 |
| (2,416) | 1:67:A:THR:HG21 | 1:86:A:PRO:HG3 | 8 | 0.28 | 0.09 | 0.32 |
| (2,416) | 1:67:A:THR:HG22 | 1:86:A:PRO:HG3 | 8 | 0.28 | 0.09 | 0.32 |
| (2,416) | 1:67:A:THR:HG23 | 1:86:A:PRO:HG3 | 8 | 0.28 | 0.09 | 0.32 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 8 | 0.22 | 0.03 | 0.24 |
| (1,27) | 1:48:A:GLN:HG2 | 1:48:A:GLN:H | 8 | 0.22 | 0.03 | 0.24 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 8 | 0.22 | 0.08 | 0.19 |
| (2,1044) | 1:47:A:ILE:HD12 | 1:19:A:CYS:H | 8 | 0.22 | 0.08 | 0.19 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 8 | 0.15 | 0.0 | 0.15 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 8 | 0.13 | 0.01 | 0.14 |
| (2,267) | 1:36:A:LEU:HD11 | 1:36:A:LEU:HA | 7 | 1.54 | 0.59 | 1.79 |
| (2,267) | 1:36:A:LEU:HD13 | 1:36:A:LEU:HA | 7 | 1.54 | 0.59 | 1.79 |
| (2,267) | 1:36:A:LEU:HD12 | 1:36:A:LEU:HA | 7 | 1.54 | 0.59 | 1.79 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 7 | 1.01 | 0.57 | 1.42 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 7 | 0.91 | 0.16 | 0.96 |
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 7 | 0.84 | 0.58 | 0.64 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG23 | 7 | 0.58 | 0.25 | 0.68 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG22 | 7 | 0.58 | 0.25 | 0.68 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG21 | 7 | 0.58 | 0.25 | 0.68 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 7 | 0.57 | 0.48 | 0.26 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD22 | 7 | 0.56 | 0.03 | 0.56 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD23 | 7 | 0.56 | 0.03 | 0.56 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 7 | 0.51 | 0.01 | 0.5 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG23 | 7 | 0.43 | 0.16 | 0.46 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG21 | 7 | 0.43 | 0.16 | 0.46 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG22 | 7 | 0.43 | 0.16 | 0.46 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 7 | 0.39 | 0.06 | 0.4 |
| (1,16) | 1:7:A:LYS:HE2 | 1:7:A:LYS:HG3 | 7 | 0.39 | 0.06 | 0.4 |
| (2,29) | 1:69:A:THR:HG21 | 1:84:A:CYS:HB2 | 7 | 0.29 | 0.12 | 0.21 |
| (2,29) | 1:69:A:THR:HG23 | 1:84:A:CYS:HB2 | 7 | 0.29 | 0.12 | 0.21 |
| (2,369) | 1:67:A:THR:HG23 | 1:68:A:PRO:HD3 | 7 | 0.28 | 0.02 | 0.28 |
| (2,369) | 1:67:A:THR:HG22 | 1:68:A:PRO:HD3 | 7 | 0.28 | 0.02 | 0.28 |
| (2,369) | 1:67:A:THR:HG21 | 1:68:A:PRO:HD3 | 7 | 0.28 | 0.02 | 0.28 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD11 | 7 | 0.27 | 0.05 | 0.3 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD12 | 7 | 0.27 | 0.05 | 0.3 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD13 | 7 | 0.27 | 0.05 | 0.3 |
| (2,1163) | 1:50:A:THR:HG23 | 1:20:A:ASP:H | 7 | 0.26 | 0.07 | 0.26 |
| (2,1163) | 1:50:A:THR:HG21 | 1:20:A:ASP:H | 7 | 0.26 | 0.07 | 0.26 |
| (2,1163) | 1:50:A:THR:HG22 | 1:20:A:ASP:H | 7 | 0.26 | 0.07 | 0.26 |
| (2,1292) | 1:67:A:THR:HG22 | 1:21:A:THR:H | 7 | 0.22 | 0.07 | 0.24 |
| (2,1292) | 1:67:A:THR:HG21 | 1:21:A:THR:H | 7 | 0.22 | 0.07 | 0.24 |
| (2,1292) | 1:67:A:THR:HG23 | 1:21:A:THR:H | 7 | 0.22 | 0.07 | 0.24 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB3 | 7 | 0.2 | 0.03 | 0.21 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB2 | 7 | 0.2 | 0.03 | 0.21 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB1 | 7 | 0.2 | 0.03 | 0.21 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 7 | 0.2 | 0.03 | 0.21 |
| (2,484) | 1:87:A:ILE:HG21 | 1:88:A:PRO:HD2 | 7 | 0.18 | 0.06 | 0.16 |
| (2,484) | 1:87:A:ILE:HG23 | 1:88:A:PRO:HD2 | 7 | 0.18 | 0.06 | 0.16 |
| (2,484) | 1:87:A:ILE:HG22 | 1:88:A:PRO:HD2 | 7 | 0.18 | 0.06 | 0.16 |
| (2,720) | 1:82:A:ILE:HG21 | 1:44:A:GLN:HA | 7 | 0.18 | 0.05 | 0.19 |
| (2,720) | 1:82:A:ILE:HG23 | 1:44:A:GLN:HA | 7 | 0.18 | 0.05 | 0.19 |
| (2,720) | 1:82:A:ILE:HG22 | 1:44:A:GLN:HA | 7 | 0.18 | 0.05 | 0.19 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 7 | 0.14 | 0.04 | 0.13 |
| (2,889) | 1:47:A:ILE:HD13 | 1:19:A:CYS:HA | 7 | 0.14 | 0.05 | 0.11 |
| (2,889) | 1:47:A:ILE:HD11 | 1:19:A:CYS:HA | 7 | 0.14 | 0.05 | 0.11 |
| (2,889) | 1:47:A:ILE:HD12 | 1:19:A:CYS:HA | 7 | 0.14 | 0.05 | 0.11 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 7 | 0.14 | 0.02 | 0.13 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 7 | 0.13 | 0.01 | 0.13 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 6 | 0.74 | 0.28 | 0.71 |
| (2,415) | 1:45:A:VAL:HG13 | 1:45:A:VAL:HA | 6 | 0.68 | 0.02 | 0.68 |
| (2,415) | 1:45:A:VAL:HG11 | 1:45:A:VAL:HA | 6 | 0.68 | 0.02 | 0.68 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,415) | 1:45:A:VAL:HG12 | 1:45:A:VAL:HA | 6 | 0.68 | 0.02 | 0.68 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 6 | 0.62 | 0.03 | 0.62 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 6 | 0.53 | 0.29 | 0.53 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 6 | 0.51 | 0.0 | 0.51 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 6 | 0.49 | 0.02 | 0.49 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG23 | 6 | 0.48 | 0.12 | 0.48 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG22 | 6 | 0.48 | 0.12 | 0.48 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG21 | 6 | 0.48 | 0.12 | 0.48 |
| (2,151) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HA | 6 | 0.46 | 0.02 | 0.47 |
| (2,151) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HA | 6 | 0.46 | 0.02 | 0.47 |
| (2,828) | 1:60:A:ILE:HD12 | 1:64:A:CYS:HB3 | 6 | 0.4 | 0.04 | 0.4 |
| (2,828) | 1:60:A:ILE:HD13 | 1:64:A:CYS:HB3 | 6 | 0.4 | 0.04 | 0.4 |
| (2,1124) | 1:41:A:VAL:HG23 | 1:44:A:GLN:HE22 | 6 | 0.3 | 0.16 | 0.26 |
| (2,1124) | 1:41:A:VAL:HG22 | 1:44:A:GLN:HE22 | 6 | 0.3 | 0.16 | 0.26 |
| (2,1124) | 1:41:A:VAL:HG21 | 1:44:A:GLN:HE22 | 6 | 0.3 | 0.16 | 0.26 |
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 6 | 0.3 | 0.09 | 0.28 |
| (2,439) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HB3 | 6 | 0.3 | 0.04 | 0.3 |
| (2,439) | 1:60:A:ILE:HG21 | 1:61:A:GLU:HB3 | 6 | 0.3 | 0.04 | 0.3 |
| (2,439) | 1:60:A:ILE:HG23 | 1:61:A:GLU:HB3 | 6 | 0.3 | 0.04 | 0.3 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 6 | 0.27 | 0.01 | 0.28 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 6 | 0.27 | 0.1 | 0.26 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 6 | 0.27 | 0.02 | 0.27 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 6 | 0.26 | 0.12 | 0.21 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 6 | 0.26 | 0.02 | 0.26 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 6 | 0.24 | 0.18 | 0.16 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 6 | 0.23 | 0.14 | 0.18 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 6 | 0.22 | 0.0 | 0.22 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 6 | 0.21 | 0.05 | 0.2 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD13 | 6 | 0.18 | 0.03 | 0.18 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD11 | 6 | 0.18 | 0.03 | 0.18 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD12 | 6 | 0.18 | 0.03 | 0.18 |
| (2,769) | 1:74:A:VAL:HG23 | 1:78:A:GLY:HA2 | 6 | 0.17 | 0.03 | 0.18 |
| (2,769) | 1:74:A:VAL:HG22 | 1:78:A:GLY:HA2 | 6 | 0.17 | 0.03 | 0.18 |
| (2,769) | 1:74:A:VAL:HG21 | 1:78:A:GLY:HA2 | 6 | 0.17 | 0.03 | 0.18 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 6 | 0.15 | 0.02 | 0.15 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 6 | 0.14 | 0.02 | 0.15 |
| (1,5) | 1:45:A:VAL:HG21 | 1:45:A:VAL:HB | 6 | 0.1 | 0.0 | 0.1 |
| (1,5) | 1:45:A:VAL:HG22 | 1:45:A:VAL:HB | 6 | 0.1 | 0.0 | 0.1 |
| (1,5) | 1:45:A:VAL:HG11 | 1:45:A:VAL:HB | 6 | 0.1 | 0.0 | 0.1 |
| (2,686) | 1:63:A:GLU:HG3 | 1:64:A:CYS:HB3 | 5 | 1.45 | 0.11 | 1.42 |
| (2,573) | 1:27:A:LYS:HA | 1:27:A:LYS:HD3 | 5 | 0.95 | 0.16 | 0.85 |
| (2,289) | 1:23:A:LYS:HB3 | 1:20:A:ASP:HB2 | 5 | 0.68 | 0.22 | 0.78 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,504) | 1:7:A:LYS:HD3 | 1:7:A:LYS:HA | 5 | 0.65 | 0.11 | 0.68 |
| (2,906) | 1:7:A:LYS:HG3 | 1:8:A:THR:HA | 5 | 0.65 | 0.26 | 0.54 |
| (2,1223) | 1:27:A:LYS:HE3 | 1:27:A:LYS:H | 5 | 0.64 | 0.16 | 0.66 |
| (2,1181) | 1:79:A:LEU:HD22 | 1:51:A:GLN:H | 5 | 0.51 | 0.17 | 0.58 |
| (2,1181) | 1:79:A:LEU:HD21 | 1:51:A:GLN:H | 5 | 0.51 | 0.17 | 0.58 |
| (2,451) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB2 | 5 | 0.5 | 0.14 | 0.55 |
| (2,452) | 1:72:A:GLU:H | 1:72:A:GLU:HB3 | 5 | 0.49 | 0.16 | 0.57 |
| (2,1213) | 1:45:A:VAL:HG22 | 1:83:A:ASN:H | 5 | 0.42 | 0.2 | 0.51 |
| (2,1213) | 1:45:A:VAL:HG23 | 1:83:A:ASN:H | 5 | 0.42 | 0.2 | 0.51 |
| (2,1122) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE22 | 5 | 0.29 | 0.07 | 0.28 |
| (2,1122) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE22 | 5 | 0.29 | 0.07 | 0.28 |
| (2,124) | 1:86:A:PRO:HG3 | 1:86:A:PRO:HA | 5 | 0.27 | 0.09 | 0.24 |
| (2,713) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB2 | 5 | 0.25 | 0.07 | 0.23 |
| (2,713) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB2 | 5 | 0.25 | 0.07 | 0.23 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD22 | 5 | 0.22 | 0.03 | 0.22 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD21 | 5 | 0.22 | 0.03 | 0.22 |
| (2,57) | 1:86:A:PRO:HG3 | 1:85:A:THR:HA | 5 | 0.2 | 0.04 | 0.19 |
| (2,1199) | 1:56:A:ILE:HG12 | 1:57:A:GLY:H | 5 | 0.19 | 0.03 | 0.2 |
| (2,809) | 1:42:A:LEU:H | 1:42:A:LEU:HG | 5 | 0.16 | 0.03 | 0.17 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG22 | 5 | 0.16 | 0.03 | 0.17 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG21 | 5 | 0.16 | 0.03 | 0.17 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG23 | 5 | 0.16 | 0.03 | 0.17 |
| (2,706) | 1:83:A:ASN:H | 1:45:A:VAL:HB | 5 | 0.14 | 0.01 | 0.15 |
| (2,589) | 1:15:A:LYS:H | 1:14:A:GLY:HA2 | 5 | 0.14 | 0.04 | 0.13 |
| (2,152) | 1:51:A:GLN:HE22 | 1:60:A:ILE:HA | 5 | 0.14 | 0.04 | 0.13 |
| (2,1119) | 1:80:A:VAL:HG13 | 1:80:A:VAL:H | 5 | 0.13 | 0.02 | 0.12 |
| (2,1119) | 1:80:A:VAL:HG11 | 1:80:A:VAL:H | 5 | 0.13 | 0.02 | 0.12 |
| (2,1119) | 1:80:A:VAL:HG12 | 1:80:A:VAL:H | 5 | 0.13 | 0.02 | 0.12 |
| (2,1189) | 1:54:A:LEU:H | 1:54:A:LEU:HA | 5 | 0.12 | 0.02 | 0.11 |
| (2,694) | 1:78:A:GLY:HA3 | 1:74:A:VAL:HB | 5 | 0.12 | 0.01 | 0.11 |
| (2,1024) | 1:85:A:THR:HG23 | 1:85:A:THR:H | 5 | 0.11 | 0.01 | 0.11 |
| (2,1024) | 1:85:A:THR:HG21 | 1:85:A:THR:H | 5 | 0.11 | 0.01 | 0.11 |
| (2,1024) | 1:85:A:THR:HG22 | 1:85:A:THR:H | 5 | 0.11 | 0.01 | 0.11 |
| (2,941) | 1:48:A:GLN:HE22 | 1:49:A:CYS:H | 4 | 1.07 | 0.04 | 1.09 |
| (2,805) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HG3 | 4 | 0.92 | 0.27 | 0.86 |
| (2,825) | 1:8:A:THR:HG23 | 1:10:A:SER:HB3 | 4 | 0.52 | 0.37 | 0.4 |
| (2,825) | 1:8:A:THR:HG22 | 1:10:A:SER:HB3 | 4 | 0.52 | 0.37 | 0.4 |
| (2,404) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HG2 | 4 | 0.48 | 0.35 | 0.36 |
| (2,404) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HG2 | 4 | 0.48 | 0.35 | 0.36 |
| (2,404) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HG2 | 4 | 0.48 | 0.35 | 0.36 |
| (2,907) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HG3 | 4 | 0.45 | 0.05 | 0.43 |
| (2,907) | 1:60:A:ILE:HG21 | 1:61:A:GLU:HG3 | 4 | 0.45 | 0.05 | 0.43 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (2,453) | 1:73:A:ASP:H | 1:72:A:GLU:HB3 | 4 | 0.41 | 0.16 | 0.48 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB3 | 4 | 0.4 | 0.17 | 0.32 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB2 | 4 | 0.4 | 0.17 | 0.32 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB1 | 4 | 0.4 | 0.17 | 0.32 |
| (2,1131) | 1:23:A:LYS:HG3 | 1:22:A:ASN:H | 4 | 0.36 | 0.21 | 0.27 |
| (2,932) | 1:43:A:ASP:HB3 | 1:43:A:ASP:H | 4 | 0.35 | 0.02 | 0.35 |
| (2,328) | 1:72:A:GLU:HG2 | 1:83:A:ASN:HB2 | 4 | 0.34 | 0.3 | 0.18 |
| (2,448) | 1:43:A:ASP:HA | 1:43:A:ASP:HB2 | 4 | 0.33 | 0.01 | 0.34 |
| (2,966) | 1:43:A:ASP:HB3 | 1:42:A:LEU:H | 4 | 0.31 | 0.1 | 0.32 |
| (2,754) | 1:5:A:GLU:H | 1:5:A:GLU:HG2 | 4 | 0.29 | 0.12 | 0.32 |
| (2,939) | 1:79:A:LEU:HB2 | 1:49:A:CYS:H | 4 | 0.21 | 0.09 | 0.2 |
| (2,409) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HB3 | 4 | 0.13 | 0.01 | 0.13 |
| (2,551) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB3 | 4 | 0.13 | 0.01 | 0.13 |
| (2,609) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HG2 | 4 | 0.12 | 0.04 | 0.11 |
| (2,830) | 1:72:A:GLU:H | 1:72:A:GLU:HG3 | 4 | 0.12 | 0.01 | 0.12 |
| (2,949) | 1:74:A:VAL:HG23 | 1:71:A:CYS:H | 3 | 2.5 | 0.19 | 2.52 |
| (2,949) | 1:74:A:VAL:HG22 | 1:71:A:CYS:H | 3 | 2.5 | 0.19 | 2.52 |
| (2,310) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA2 | 3 | 2.27 | 0.02 | 2.26 |
| (2,310) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA2 | 3 | 2.27 | 0.02 | 2.26 |
| (2,637) | 1:74:A:VAL:HG23 | 1:71:A:CYS:HB3 | 3 | 2.15 | 0.09 | 2.1 |
| (2,637) | 1:74:A:VAL:HG22 | 1:71:A:CYS:HB3 | 3 | 2.15 | 0.09 | 2.1 |
| (2,34) | 1:74:A:VAL:HG23 | 1:71:A:CYS:HB2 | 3 | 2.06 | 0.12 | 2.01 |
| (2,34) | 1:74:A:VAL:HG22 | 1:71:A:CYS:HB2 | 3 | 2.06 | 0.12 | 2.01 |
| (2,1166) | 1:23:A:LYS:HB2 | 1:20:A:ASP:H | 3 | 0.97 | 0.01 | 0.97 |
| (2,383) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB2 | 3 | 0.83 | 0.03 | 0.85 |
| (2,1102) | 1:48:A:GLN:H | 1:23:A:LYS:HB2 | 3 | 0.8 | 0.06 | 0.82 |
| (2,1273) | 1:24:A:LYS:H | 1:24:A:LYS:HD3 | 3 | 0.76 | 0.39 | 1.04 |
| (2,147) | 1:24:A:LYS:H | 1:24:A:LYS:HB2 | 3 | 0.56 | 0.07 | 0.61 |
| (2,865) | 1:74:A:VAL:H | 1:15:A:LYS:HE3 | 3 | 0.52 | 0.2 | 0.45 |
| (2,843) | 1:41:A:VAL:HG21 | 1:38:A:THR:HA | 3 | 0.42 | 0.01 | 0.42 |
| (2,722) | 1:87:A:ILE:HG21 | 1:70:A:CYS:HB3 | 3 | 0.39 | 0.11 | 0.46 |
| (2,722) | 1:87:A:ILE:HG23 | 1:70:A:CYS:HB3 | 3 | 0.39 | 0.11 | 0.46 |
| (2,722) | 1:87:A:ILE:HG22 | 1:70:A:CYS:HB3 | 3 | 0.39 | 0.11 | 0.46 |
| (2,661) | 1:74:A:VAL:HG11 | 1:78:A:GLY:HA3 | 3 | 0.38 | 0.13 | 0.41 |
| (2,661) | 1:74:A:VAL:HG13 | 1:78:A:GLY:HA3 | 3 | 0.38 | 0.13 | 0.41 |
| (2,577) | 1:16:A:LEU:HD12 | 1:11:A:CYS:HB3 | 3 | 0.37 | 0.08 | 0.33 |
| (2,577) | 1:16:A:LEU:HD13 | 1:11:A:CYS:HB3 | 3 | 0.37 | 0.08 | 0.33 |
| (2,577) | 1:16:A:LEU:HD11 | 1:11:A:CYS:HB3 | 3 | 0.37 | 0.08 | 0.33 |
| (2,879) | 1:59:A:ALA:H | 1:62:A:ASP:HB3 | 3 | 0.33 | 0.06 | 0.3 |
| (2,814) | 1:24:A:LYS:H | 1:23:A:LYS:HB3 | 3 | 0.26 | 0.02 | 0.26 |
| (2,666) | 1:84:A:CYS:HB3 | 1:71:A:CYS:HA | 3 | 0.24 | 0.01 | 0.25 |
| (1,7) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB3 | 3 | 0.24 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB3 | 3 | 0.24 | 0.07 | 0.24 |
| (1,7) | 1:41:A:VAL:HG13 | 1:40:A:ASP:HB3 | 3 | 0.24 | 0.07 | 0.24 |
| (2,568) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HB2 | 3 | 0.23 | 0.06 | 0.23 |
| (2,434) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HG2 | 3 | 0.21 | 0.0 | 0.21 |
| (2,537) | 1:25:A:VAL:HG21 | 1:48:A:GLN:HA | 3 | 0.2 | 0.07 | 0.19 |
| (2,537) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HA | 3 | 0.2 | 0.07 | 0.19 |
| (2,821) | 1:11:A:CYS:H | 1:10:A:SER:HB3 | 3 | 0.19 | 0.02 | 0.18 |
| (2,819) | 1:35:A:LEU:H | 1:35:A:LEU:HG | 3 | 0.17 | 0.01 | 0.16 |
| (2,183) | 1:23:A:LYS:HG3 | 1:20:A:ASP:HB2 | 3 | 0.16 | 0.02 | 0.16 |
| (2,626) | 1:52:A:ILE:HB | 1:64:A:CYS:HB2 | 3 | 0.14 | 0.02 | 0.14 |
| (2,1209) | 1:26:A:GLN:H | 1:25:A:VAL:HB | 3 | 0.14 | 0.01 | 0.13 |
| (2,174) | 1:83:A:ASN:H | 1:82:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.14 |
| (2,174) | 1:83:A:ASN:H | 1:82:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.14 |
| (2,257) | 1:59:A:ALA:H | 1:58:A:ILE:HB | 3 | 0.13 | 0.02 | 0.12 |
| (2,129) | 1:79:A:LEU:HG | 1:76:A:ASP:HB2 | 3 | 0.12 | 0.03 | 0.11 |
| (2,153) | 1:51:A:GLN:HE21 | 1:60:A:ILE:HA | 3 | 0.11 | 0.0 | 0.11 |
| (2,165) | 1:42:A:LEU:HA | 1:42:A:LEU:HB3 | 3 | 0.11 | 0.0 | 0.11 |
| (2,869) | 1:52:A:ILE:HG13 | 1:51:A:GLN:HA | 2 | 1.3 | 0.01 | 1.3 |
| (2,792) | 1:82:A:ILE:HG13 | 1:73:A:ASP:HB3 | 2 | 1.06 | 0.06 | 1.06 |
| (2,313) | 1:52:A:ILE:HB | 1:52:A:ILE:HD13 | 2 | 0.66 | 0.01 | 0.66 |
| (2,1046) | 1:13:A:THR:HG21 | 1:12:A:ASN:HD22 | 2 | 0.57 | 0.02 | 0.57 |
| (2,1046) | 1:13:A:THR:HG22 | 1:12:A:ASN:HD22 | 2 | 0.57 | 0.02 | 0.57 |
| (2,1196) | 1:35:A:LEU:H | 1:34:A:GLY:HA3 | 2 | 0.4 | 0.0 | 0.4 |
| (2,1072) | 1:31:A:GLU:H | 1:31:A:GLU:HG2 | 2 | 0.36 | 0.19 | 0.36 |
| (2,759) | 1:75:A:GLU:HA | 1:75:A:GLU:HG2 | 2 | 0.34 | 0.05 | 0.34 |
| (2,1221) | 1:27:A:LYS:H | 1:27:A:LYS:HB2 | 2 | 0.33 | 0.16 | 0.33 |
| (2,1153) | 1:32:A:GLU:H | 1:32:A:GLU:HG3 | 2 | 0.32 | 0.11 | 0.32 |
| (2,624) | 1:74:A:VAL:HG11 | 1:78:A:GLY:HA2 | 2 | 0.27 | 0.02 | 0.27 |
| (2,624) | 1:74:A:VAL:HG13 | 1:78:A:GLY:HA2 | 2 | 0.27 | 0.02 | 0.27 |
| (2,1076) | 1:29:A:THR:H | 1:28:A:SER:HA | 2 | 0.22 | 0.02 | 0.22 |
| (2,516) | 1:31:A:GLU:HA | 1:31:A:GLU:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (2,1083) | 1:26:A:GLN:HB2 | 1:26:A:GLN:HE21 | 2 | 0.18 | 0.04 | 0.18 |
| (2,1159) | 1:47:A:ILE:HG21 | 1:46:A:ALA:H | 2 | 0.18 | 0.04 | 0.18 |
| (2,1159) | 1:47:A:ILE:HG22 | 1:46:A:ALA:H | 2 | 0.18 | 0.04 | 0.18 |
| (2,7) | 1:12:A:ASN:HB2 | 1:12:A:ASN:HA | 2 | 0.17 | 0.02 | 0.17 |
| (2,758) | 1:76:A:ASP:H | 1:75:A:GLU:HG3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,857) | 1:90:A:ILE:HG12 | 1:88:A:PRO:HG3 | 2 | 0.16 | 0.02 | 0.16 |
| (2,423) | 1:54:A:LEU:H | 1:54:A:LEU:HD13 | 2 | 0.14 | 0.02 | 0.14 |
| (2,423) | 1:54:A:LEU:H | 1:54:A:LEU:HD11 | 2 | 0.14 | 0.02 | 0.14 |
| (2,898) | 1:90:A:ILE:H | 1:88:A:PRO:HD2 | 2 | 0.14 | 0.01 | 0.14 |
| (2,387) | 1:66:A:ASN:HD21 | 1:66:A:ASN:HA | 2 | 0.13 | 0.01 | 0.13 |
| (2,562) | 1:53:A:PRO:HD2 | 1:52:A:ILE:HB | 2 | 0.13 | 0.01 | 0.13 |

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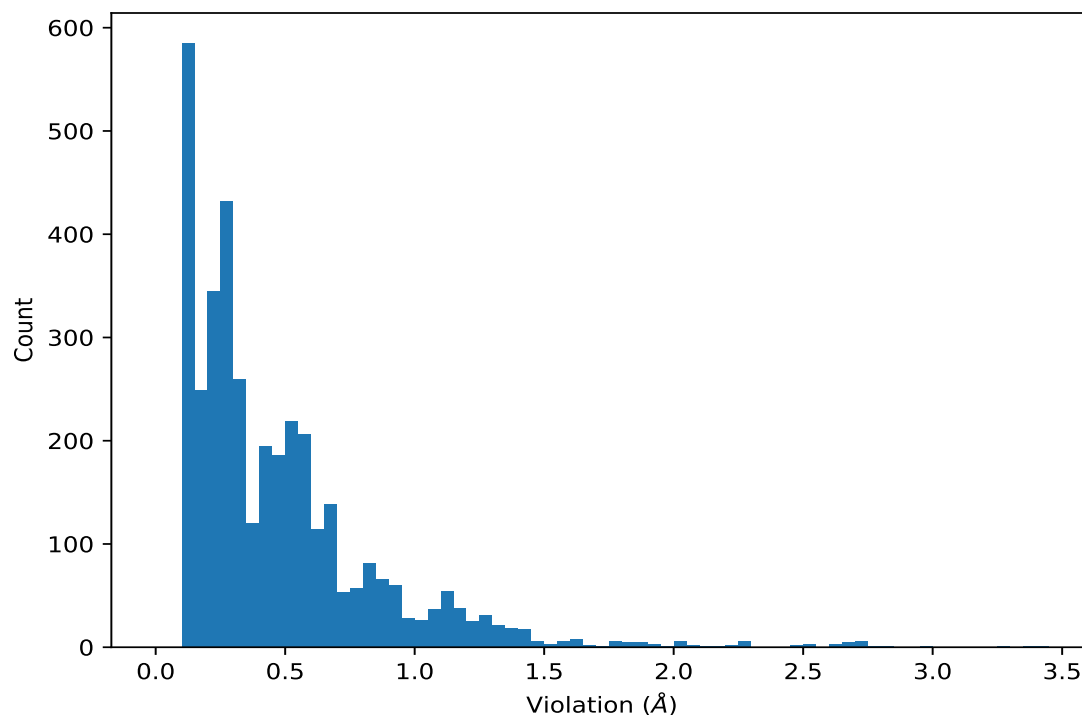
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (2,681) | 1:60:A:ILE:HD12 | 1:18:A:CYS:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (2,681) | 1:60:A:ILE:HD11 | 1:18:A:CYS:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (2,877) | 1:80:A:VAL:H | 1:78:A:GLY:HA3 | 2 | 0.12 | 0.02 | 0.12 |
| (2,1077) | 1:28:A:SER:HB2 | 1:29:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (2,904) | 1:16:A:LEU:HG | 1:11:A:CYS:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1186) | 1:87:A:ILE:H | 1:88:A:PRO:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,797) | 1:25:A:VAL:H | 1:24:A:LYS:HB2 | 2 | 0.11 | 0.01 | 0.11 |
| (2,913) | 1:61:A:GLU:H | 1:61:A:GLU:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (2,1278) | 1:38:A:THR:HA | 1:41:A:VAL:H | 2 | 0.11 | 0.0 | 0.11 |
| (2,628) | 1:88:A:PRO:HD2 | 1:88:A:PRO:HB3 | 2 | 0.1 | 0.0 | 0.1 |

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) |
|----------|-----------------|-----------------|----------|---------------|
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 18 | 3.41 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 15 | 3.36 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 8 | 3.3 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 16 | 2.96 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 8 | 2.83 |
| (2,459) | 1:45:A:VAL:HG13 | 1:44:A:GLN:HA | 17 | 2.75 |
| (2,949) | 1:74:A:VAL:HG22 | 1:71:A:CYS:H | 18 | 2.72 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 6 | 2.71 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 15 | 2.71 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 16 | 2.71 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 18 | 2.71 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 1 | 2.7 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 7 | 2.69 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 5 | 2.68 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 19 | 2.68 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 9 | 2.67 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 12 | 2.67 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 3 | 2.65 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 14 | 2.64 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 2 | 2.61 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 14 | 2.52 |
| (2,949) | 1:74:A:VAL:HG23 | 1:71:A:CYS:H | 15 | 2.52 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 2 | 2.51 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 13 | 2.45 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 19 | 2.45 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD13 | 1 | 2.3 |
| (2,310) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA2 | 15 | 2.3 |
| (2,637) | 1:74:A:VAL:HG22 | 1:71:A:CYS:HB3 | 18 | 2.27 |
| (2,310) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA2 | 18 | 2.26 |
| (2,949) | 1:74:A:VAL:HG23 | 1:71:A:CYS:H | 8 | 2.25 |
| (2,310) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA2 | 8 | 2.25 |
| (2,34) | 1:74:A:VAL:HG22 | 1:71:A:CYS:HB2 | 18 | 2.22 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD12 | 8 | 2.2 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 1 | 2.19 |
| (2,637) | 1:74:A:VAL:HG23 | 1:71:A:CYS:HB3 | 8 | 2.1 |
| (2,637) | 1:74:A:VAL:HG23 | 1:71:A:CYS:HB3 | 15 | 2.08 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD12 | 6 | 2.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 16 | 2.05 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD11 | 14 | 2.05 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 20 | 2.03 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD11 | 4 | 2.01 |
| (2,34) | 1:74:A:VAL:HG23 | 1:71:A:CYS:HB2 | 15 | 2.01 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD12 | 10 | 2.0 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 13 | 1.99 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 5 | 1.94 |
| (2,34) | 1:74:A:VAL:HG23 | 1:71:A:CYS:HB2 | 8 | 1.94 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 3 | 1.93 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 2 | 1.89 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 16 | 1.85 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 17 | 1.85 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG21 | 18 | 1.85 |
| (2,267) | 1:36:A:LEU:HD13 | 1:36:A:LEU:HA | 4 | 1.85 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 8 | 1.83 |
| (2,267) | 1:36:A:LEU:HD11 | 1:36:A:LEU:HA | 10 | 1.83 |
| (2,543) | 1:79:A:LEU:HD21 | 1:50:A:THR:HA | 8 | 1.82 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 2 | 1.82 |
| (2,267) | 1:36:A:LEU:HD11 | 1:36:A:LEU:HA | 2 | 1.8 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 7 | 1.79 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 18 | 1.79 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 7 | 1.79 |
| (2,267) | 1:36:A:LEU:HD12 | 1:36:A:LEU:HA | 15 | 1.79 |
| (2,267) | 1:36:A:LEU:HD13 | 1:36:A:LEU:HA | 19 | 1.77 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD12 | 9 | 1.76 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 4 | 1.72 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 4 | 1.68 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 16 | 1.66 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 10 | 1.65 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 5 | 1.65 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 1 | 1.65 |
| (2,267) | 1:36:A:LEU:HD13 | 1:36:A:LEU:HA | 9 | 1.64 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 20 | 1.63 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 10 | 1.62 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 20 | 1.62 |
| (2,686) | 1:63:A:GLU:HG3 | 1:64:A:CYS:HB3 | 14 | 1.61 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 7 | 1.59 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 15 | 1.58 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 18 | 1.58 |
| (2,686) | 1:63:A:GLU:HG3 | 1:64:A:CYS:HB3 | 17 | 1.56 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 6 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 9 | 1.55 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 13 | 1.51 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 16 | 1.5 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG21 | 10 | 1.5 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 1 | 1.48 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 12 | 1.48 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 8 | 1.47 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 20 | 1.47 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 2 | 1.46 |
| (2,112) | 1:67:A:THR:HG21 | 1:68:A:PRO:HG3 | 14 | 1.46 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 10 | 1.45 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 16 | 1.45 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 6 | 1.45 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 18 | 1.45 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 9 | 1.44 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 9 | 1.44 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 19 | 1.44 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 12 | 1.43 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 10 | 1.43 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 1 | 1.42 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 16 | 1.42 |
| (2,686) | 1:63:A:GLU:HG3 | 1:64:A:CYS:HB3 | 19 | 1.42 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 18 | 1.42 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 2 | 1.42 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 11 | 1.41 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 13 | 1.41 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 20 | 1.41 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 15 | 1.4 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 17 | 1.4 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 6 | 1.4 |
| (2,508) | 1:5:A:GLU:HB2 | 1:59:A:ALA:HA | 11 | 1.4 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 12 | 1.4 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG23 | 5 | 1.39 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 14 | 1.39 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 10 | 1.39 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 1 | 1.38 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 3 | 1.38 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 4 | 1.37 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 10 | 1.37 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 8 | 1.37 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 11 | 1.37 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 7 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 19 | 1.35 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 4 | 1.35 |
| (2,112) | 1:67:A:THR:HG21 | 1:68:A:PRO:HG3 | 19 | 1.35 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 3 | 1.34 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 4 | 1.34 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 7 | 1.34 |
| (2,686) | 1:63:A:GLU:HG3 | 1:64:A:CYS:HB3 | 11 | 1.34 |
| (2,686) | 1:63:A:GLU:HG3 | 1:64:A:CYS:HB3 | 15 | 1.34 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 10 | 1.34 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 3 | 1.33 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 9 | 1.33 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 19 | 1.33 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG21 | 6 | 1.32 |
| (2,848) | 1:89:A:LEU:HB3 | 1:90:A:ILE:HG22 | 18 | 1.32 |
| (2,428) | 1:59:A:ALA:HB2 | 1:62:A:ASP:HB3 | 12 | 1.32 |
| (2,940) | 1:79:A:LEU:HD21 | 1:49:A:CYS:H | 8 | 1.31 |
| (2,869) | 1:52:A:ILE:HG13 | 1:51:A:GLN:HA | 19 | 1.31 |
| (2,805) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HG3 | 19 | 1.31 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 2 | 1.3 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 9 | 1.3 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 14 | 1.3 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 20 | 1.3 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 8 | 1.3 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG23 | 16 | 1.3 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 8 | 1.29 |
| (2,869) | 1:52:A:ILE:HG13 | 1:51:A:GLN:HA | 15 | 1.29 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 15 | 1.29 |
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 14 | 1.29 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 3 | 1.28 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 20 | 1.28 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 12 | 1.27 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 9 | 1.27 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG23 | 15 | 1.27 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 18 | 1.26 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 4 | 1.26 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 6 | 1.26 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 12 | 1.26 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 3 | 1.26 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD23 | 15 | 1.26 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 19 | 1.26 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 20 | 1.26 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 20 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 9 | 1.26 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 6 | 1.25 |
| (2,1225) | 1:45:A:VAL:HG12 | 1:45:A:VAL:H | 7 | 1.25 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 16 | 1.25 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 19 | 1.25 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 14 | 1.25 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 19 | 1.25 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 6 | 1.25 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 16 | 1.25 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 15 | 1.25 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 1 | 1.25 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 17 | 1.25 |
| (2,112) | 1:67:A:THR:HG21 | 1:68:A:PRO:HG3 | 15 | 1.25 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 1 | 1.24 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 19 | 1.24 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 7 | 1.24 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD23 | 11 | 1.24 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 12 | 1.24 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD23 | 17 | 1.24 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG23 | 2 | 1.24 |
| (2,1225) | 1:45:A:VAL:HG11 | 1:45:A:VAL:H | 17 | 1.23 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 18 | 1.23 |
| (2,573) | 1:27:A:LYS:HA | 1:27:A:LYS:HD3 | 6 | 1.23 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 2 | 1.23 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 13 | 1.23 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 18 | 1.23 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 5 | 1.22 |
| (2,1225) | 1:45:A:VAL:HG11 | 1:45:A:VAL:H | 15 | 1.22 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 5 | 1.22 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 4 | 1.22 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 19 | 1.22 |
| (2,112) | 1:67:A:THR:HG21 | 1:68:A:PRO:HG3 | 3 | 1.22 |
| (2,1225) | 1:45:A:VAL:HG13 | 1:45:A:VAL:H | 1 | 1.21 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 7 | 1.21 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 7 | 1.21 |
| (2,112) | 1:67:A:THR:HG21 | 1:68:A:PRO:HG3 | 1 | 1.21 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 5 | 1.21 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 18 | 1.21 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 3 | 1.2 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 10 | 1.2 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 6 | 1.2 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 10 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 10 | 1.2 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG23 | 1 | 1.2 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG23 | 6 | 1.2 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 12 | 1.2 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 6 | 1.2 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD12 | 6 | 1.2 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 3 | 1.19 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 18 | 1.19 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 11 | 1.19 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 4 | 1.19 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG21 | 16 | 1.19 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 8 | 1.19 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 20 | 1.19 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 17 | 1.19 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 18 | 1.19 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 13 | 1.19 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 17 | 1.19 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 15 | 1.18 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 12 | 1.17 |
| (2,682) | 1:17:A:ALA:HB2 | 1:18:A:CYS:HB3 | 5 | 1.17 |
| (2,682) | 1:17:A:ALA:HB2 | 1:18:A:CYS:HB3 | 17 | 1.17 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 5 | 1.16 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 16 | 1.16 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 19 | 1.16 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 4 | 1.16 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 12 | 1.16 |
| (2,682) | 1:17:A:ALA:HB2 | 1:18:A:CYS:HB3 | 15 | 1.16 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 14 | 1.16 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG21 | 7 | 1.16 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG21 | 11 | 1.16 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 7 | 1.16 |
| (2,112) | 1:67:A:THR:HG23 | 1:68:A:PRO:HG3 | 16 | 1.16 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 8 | 1.16 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 13 | 1.16 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 12 | 1.15 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 8 | 1.15 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 3 | 1.15 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 13 | 1.15 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 4 | 1.15 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 1 | 1.14 |
| (2,565) | 1:42:A:LEU:HD12 | 1:42:A:LEU:HB2 | 17 | 1.14 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 3 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 20 | 1.14 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 19 | 1.13 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 6 | 1.13 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 1 | 1.13 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 6 | 1.13 |
| (2,792) | 1:82:A:ILE:HG13 | 1:73:A:ASP:HB3 | 16 | 1.13 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 14 | 1.13 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 1 | 1.13 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 11 | 1.13 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 16 | 1.13 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 18 | 1.13 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 14 | 1.13 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG23 | 19 | 1.13 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 1 | 1.13 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 19 | 1.12 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 14 | 1.12 |
| (2,906) | 1:7:A:LYS:HG3 | 1:8:A:THR:HA | 7 | 1.12 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 5 | 1.12 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 18 | 1.12 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 13 | 1.12 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 15 | 1.12 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 19 | 1.12 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG21 | 10 | 1.12 |
| (2,1255) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE21 | 19 | 1.11 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 14 | 1.11 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 1 | 1.11 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 9 | 1.11 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 15 | 1.11 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 3 | 1.11 |
| (2,825) | 1:8:A:THR:HG22 | 1:10:A:SER:HB3 | 17 | 1.11 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 2 | 1.11 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 9 | 1.11 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 16 | 1.11 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 9 | 1.11 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 16 | 1.11 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG21 | 10 | 1.11 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 12 | 1.11 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 13 | 1.11 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 4 | 1.11 |
| (2,112) | 1:67:A:THR:HG22 | 1:68:A:PRO:HG3 | 11 | 1.11 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 13 | 1.1 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 3 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,941) | 1:48:A:GLN:HE22 | 1:49:A:CYS:H | 6 | 1.1 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 6 | 1.1 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 8 | 1.1 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 14 | 1.1 |
| (2,941) | 1:48:A:GLN:HE22 | 1:49:A:CYS:H | 11 | 1.09 |
| (2,941) | 1:48:A:GLN:HE22 | 1:49:A:CYS:H | 15 | 1.09 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 5 | 1.09 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 11 | 1.09 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 2 | 1.09 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 2 | 1.08 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 10 | 1.08 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 12 | 1.08 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 4 | 1.08 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 4 | 1.08 |
| (2,404) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HG2 | 4 | 1.08 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 1 | 1.08 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 17 | 1.07 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 11 | 1.07 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 16 | 1.07 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 17 | 1.07 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 11 | 1.07 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 4 | 1.07 |
| (2,1255) | 1:82:A:ILE:HD11 | 1:44:A:GLN:HE21 | 16 | 1.06 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 17 | 1.06 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 17 | 1.06 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 9 | 1.06 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 2 | 1.06 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 5 | 1.06 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 6 | 1.06 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 7 | 1.06 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 13 | 1.05 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 8 | 1.05 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 17 | 1.05 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG22 | 17 | 1.05 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 11 | 1.05 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 13 | 1.05 |
| (2,573) | 1:27:A:LYS:HA | 1:27:A:LYS:HD3 | 16 | 1.05 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 10 | 1.05 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 13 | 1.05 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 12 | 1.05 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 18 | 1.05 |
| (2,1273) | 1:24:A:LYS:H | 1:24:A:LYS:HD3 | 3 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1273) | 1:24:A:LYS:H | 1:24:A:LYS:HD3 | 13 | 1.04 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 11 | 1.04 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 8 | 1.04 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 11 | 1.04 |
| (2,682) | 1:17:A:ALA:HB2 | 1:18:A:CYS:HB3 | 20 | 1.04 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG21 | 4 | 1.04 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 8 | 1.03 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 18 | 1.03 |
| (2,805) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HG3 | 14 | 1.02 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 1 | 1.02 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 10 | 1.02 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 1 | 1.02 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 4 | 1.02 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 9 | 1.02 |
| (2,682) | 1:17:A:ALA:HB3 | 1:18:A:CYS:HB3 | 2 | 1.01 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 1 | 1.01 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 3 | 1.01 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 9 | 1.01 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 8 | 1.01 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 2 | 1.01 |
| (2,941) | 1:48:A:GLN:HE22 | 1:49:A:CYS:H | 5 | 1.0 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 19 | 1.0 |
| (2,792) | 1:82:A:ILE:HG13 | 1:73:A:ASP:HB3 | 18 | 1.0 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 12 | 1.0 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 16 | 1.0 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 10 | 0.98 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 18 | 0.98 |
| (2,1166) | 1:23:A:LYS:HB2 | 1:20:A:ASP:H | 15 | 0.98 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 4 | 0.98 |
| (2,946) | 1:10:A:SER:HB3 | 1:9:A:GLY:H | 5 | 0.98 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 15 | 0.98 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 10 | 0.98 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 14 | 0.98 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 2 | 0.98 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 11 | 0.98 |
| (2,1255) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE21 | 1 | 0.97 |
| (2,1166) | 1:23:A:LYS:HB2 | 1:20:A:ASP:H | 14 | 0.97 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 20 | 0.97 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 19 | 0.97 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 7 | 0.97 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 13 | 0.97 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 10 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 12 | 0.97 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG21 | 13 | 0.97 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 11 | 0.96 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 18 | 0.96 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 16 | 0.96 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 1 | 0.96 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 3 | 0.96 |
| (2,428) | 1:59:A:ALA:HB3 | 1:62:A:ASP:HB3 | 10 | 0.96 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 1 | 0.96 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 16 | 0.96 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG22 | 3 | 0.96 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 9 | 0.95 |
| (2,1166) | 1:23:A:LYS:HB2 | 1:20:A:ASP:H | 20 | 0.95 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 7 | 0.95 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 15 | 0.95 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 20 | 0.95 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 18 | 0.95 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 13 | 0.95 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 16 | 0.95 |
| (2,138) | 1:23:A:LYS:HA | 1:23:A:LYS:HD3 | 9 | 0.95 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 2 | 0.94 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 12 | 0.94 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 1 | 0.94 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 9 | 0.94 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB2 | 15 | 0.94 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 2 | 0.94 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 8 | 0.94 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 20 | 0.94 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 13 | 0.94 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 4 | 0.94 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 5 | 0.94 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 14 | 0.93 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 12 | 0.93 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 14 | 0.93 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 1 | 0.93 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 18 | 0.93 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 19 | 0.93 |
| (2,519) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HG12 | 14 | 0.93 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 5 | 0.93 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 19 | 0.93 |
| (2,397) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB3 | 12 | 0.93 |
| (2,74) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HB2 | 12 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD11 | 10 | 0.93 |
| (2,24) | 1:60:A:ILE:HD13 | 1:60:A:ILE:HG22 | 11 | 0.93 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 4 | 0.92 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 1 | 0.92 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 7 | 0.92 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 5 | 0.92 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 9 | 0.92 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 11 | 0.92 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 3 | 0.92 |
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 11 | 0.91 |
| (2,1255) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE21 | 13 | 0.91 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 18 | 0.91 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 12 | 0.91 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 5 | 0.91 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 3 | 0.91 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 8 | 0.91 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 13 | 0.91 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 20 | 0.91 |
| (2,1223) | 1:27:A:LYS:HE3 | 1:27:A:LYS:H | 12 | 0.9 |
| (2,948) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE21 | 5 | 0.9 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 2 | 0.9 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 4 | 0.9 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 10 | 0.9 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 15 | 0.9 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 17 | 0.9 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 20 | 0.9 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 14 | 0.9 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 14 | 0.9 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 1 | 0.9 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 2 | 0.89 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 7 | 0.89 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 6 | 0.89 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 20 | 0.89 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 14 | 0.89 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 15 | 0.89 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 1 | 0.89 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 3 | 0.89 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 8 | 0.89 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 13 | 0.89 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 16 | 0.89 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 19 | 0.89 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 10 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 19 | 0.89 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 7 | 0.89 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 12 | 0.89 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 8 | 0.89 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG22 | 8 | 0.89 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG23 | 19 | 0.89 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 13 | 0.88 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 1 | 0.88 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 2 | 0.88 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 17 | 0.88 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 8 | 0.88 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 12 | 0.88 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 16 | 0.88 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 17 | 0.88 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 18 | 0.88 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 20 | 0.88 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 6 | 0.88 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 12 | 0.88 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 14 | 0.88 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 9 | 0.88 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 15 | 0.88 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 19 | 0.88 |
| (2,205) | 1:74:A:VAL:HG23 | 1:15:A:LYS:HE3 | 11 | 0.88 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 11 | 0.88 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG23 | 20 | 0.88 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 18 | 0.87 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 19 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 1 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 2 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 4 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 6 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 7 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 10 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 11 | 0.87 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 19 | 0.87 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 7 | 0.87 |
| (2,596) | 1:89:A:LEU:H | 1:89:A:LEU:HB3 | 18 | 0.87 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 14 | 0.87 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 17 | 0.87 |
| (2,24) | 1:60:A:ILE:HD13 | 1:60:A:ILE:HG21 | 1 | 0.87 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG23 | 13 | 0.87 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 11 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 18 | 0.86 |
| (2,1102) | 1:48:A:GLN:H | 1:23:A:LYS:HB2 | 15 | 0.86 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 4 | 0.86 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 7 | 0.86 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 9 | 0.86 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 12 | 0.86 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 9 | 0.86 |
| (2,383) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB2 | 20 | 0.86 |
| (2,328) | 1:72:A:GLU:HG2 | 1:83:A:ASN:HB2 | 16 | 0.86 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 13 | 0.86 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG23 | 5 | 0.86 |
| (2,1255) | 1:82:A:ILE:HD11 | 1:44:A:GLN:HE21 | 7 | 0.85 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 13 | 0.85 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 8 | 0.85 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 9 | 0.85 |
| (2,682) | 1:17:A:ALA:HB1 | 1:18:A:CYS:HB3 | 7 | 0.85 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 15 | 0.85 |
| (2,573) | 1:27:A:LYS:HA | 1:27:A:LYS:HD3 | 14 | 0.85 |
| (2,383) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB2 | 14 | 0.85 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG23 | 5 | 0.85 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 12 | 0.85 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG22 | 9 | 0.85 |
| (2,24) | 1:60:A:ILE:HD13 | 1:60:A:ILE:HG21 | 18 | 0.85 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 14 | 0.84 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 12 | 0.84 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 2 | 0.84 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 11 | 0.84 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 16 | 0.84 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG23 | 19 | 0.84 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 20 | 0.84 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 4 | 0.84 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 17 | 0.84 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 18 | 0.84 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG22 | 20 | 0.84 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG23 | 15 | 0.84 |
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 20 | 0.83 |
| (2,1253) | 1:16:A:LEU:HD12 | 1:4:A:TRP:HE1 | 3 | 0.83 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 16 | 0.83 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 15 | 0.83 |
| (2,940) | 1:79:A:LEU:HD23 | 1:49:A:CYS:H | 9 | 0.83 |
| (2,918) | 1:79:A:LEU:HB2 | 1:48:A:GLN:HA | 17 | 0.83 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 17 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,573) | 1:27:A:LYS:HA | 1:27:A:LYS:HD3 | 7 | 0.83 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 8 | 0.83 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 12 | 0.83 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 2 | 0.83 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 16 | 0.83 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 7 | 0.83 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 8 | 0.83 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD13 | 12 | 0.83 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD13 | 16 | 0.83 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 8 | 0.82 |
| (2,1102) | 1:48:A:GLN:H | 1:23:A:LYS:HB2 | 14 | 0.82 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 3 | 0.82 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 6 | 0.82 |
| (2,678) | 1:70:A:CYS:HB3 | 1:11:A:CYS:HB3 | 20 | 0.82 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 3 | 0.82 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 19 | 0.82 |
| (2,289) | 1:23:A:LYS:HB3 | 1:20:A:ASP:HB2 | 8 | 0.82 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 2 | 0.82 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 4 | 0.82 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 5 | 0.82 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 9 | 0.82 |
| (2,1158) | 1:45:A:VAL:HG23 | 1:46:A:ALA:H | 9 | 0.81 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 17 | 0.81 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 1 | 0.81 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 12 | 0.81 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 3 | 0.81 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 4 | 0.81 |
| (2,573) | 1:27:A:LYS:HA | 1:27:A:LYS:HD3 | 17 | 0.81 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 7 | 0.81 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 14 | 0.81 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 11 | 0.81 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG21 | 12 | 0.81 |
| (2,428) | 1:59:A:ALA:HB1 | 1:62:A:ASP:HB3 | 2 | 0.81 |
| (2,205) | 1:74:A:VAL:HG21 | 1:15:A:LYS:HE3 | 2 | 0.81 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 17 | 0.81 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 18 | 0.81 |
| (2,24) | 1:60:A:ILE:HD13 | 1:60:A:ILE:HG21 | 16 | 0.81 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 16 | 0.8 |
| (2,892) | 1:69:A:THR:HG23 | 1:19:A:CYS:HA | 13 | 0.8 |
| (2,865) | 1:74:A:VAL:H | 1:15:A:LYS:HE3 | 20 | 0.8 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 9 | 0.8 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 17 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 15 | 0.8 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 8 | 0.8 |
| (2,289) | 1:23:A:LYS:HB3 | 1:20:A:ASP:HB2 | 3 | 0.8 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG22 | 11 | 0.8 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG23 | 17 | 0.8 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 7 | 0.8 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 3 | 0.8 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD12 | 11 | 0.8 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 2 | 0.79 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 11 | 0.79 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 4 | 0.79 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 1 | 0.79 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 15 | 0.79 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 16 | 0.79 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 4 | 0.79 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 9 | 0.79 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 20 | 0.79 |
| (2,383) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB2 | 15 | 0.79 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 5 | 0.79 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 20 | 0.79 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 6 | 0.79 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 16 | 0.79 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD13 | 3 | 0.79 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD13 | 8 | 0.79 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD12 | 17 | 0.79 |
| (2,24) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HG22 | 7 | 0.79 |
| (2,1158) | 1:45:A:VAL:HG23 | 1:46:A:ALA:H | 2 | 0.78 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 18 | 0.78 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG23 | 2 | 0.78 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 13 | 0.78 |
| (2,683) | 1:50:A:THR:HG22 | 1:18:A:CYS:HB2 | 3 | 0.78 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 16 | 0.78 |
| (2,289) | 1:23:A:LYS:HB3 | 1:20:A:ASP:HB2 | 1 | 0.78 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 4 | 0.78 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 6 | 0.78 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 12 | 0.78 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 15 | 0.78 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 1 | 0.78 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 10 | 0.78 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 12 | 0.78 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 17 | 0.77 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 2 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,504) | 1:7:A:LYS:HD3 | 1:7:A:LYS:HA | 6 | 0.77 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 7 | 0.77 |
| (2,24) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HG21 | 2 | 0.77 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 14 | 0.76 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 4 | 0.76 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 7 | 0.76 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 5 | 0.76 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 1 | 0.76 |
| (2,517) | 1:31:A:GLU:HA | 1:31:A:GLU:HG2 | 9 | 0.76 |
| (2,289) | 1:23:A:LYS:HB3 | 1:20:A:ASP:HB2 | 18 | 0.76 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 2 | 0.76 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 18 | 0.76 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD11 | 13 | 0.76 |
| (2,1253) | 1:16:A:LEU:HD12 | 1:4:A:TRP:HE1 | 7 | 0.75 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG23 | 10 | 0.75 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 17 | 0.75 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 13 | 0.75 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 19 | 0.75 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 11 | 0.75 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 16 | 0.75 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 16 | 0.75 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD11 | 5 | 0.75 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD11 | 20 | 0.75 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 15 | 0.74 |
| (2,1210) | 1:46:A:ALA:HB3 | 1:26:A:GLN:H | 4 | 0.74 |
| (2,1167) | 1:47:A:ILE:HG22 | 1:20:A:ASP:H | 13 | 0.74 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 17 | 0.74 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 10 | 0.74 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 11 | 0.74 |
| (2,630) | 1:52:A:ILE:HD11 | 1:64:A:CYS:HB3 | 19 | 0.74 |
| (2,428) | 1:59:A:ALA:HB2 | 1:62:A:ASP:HB3 | 20 | 0.74 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 12 | 0.74 |
| (2,323) | 1:69:A:THR:HG21 | 1:86:A:PRO:HD2 | 15 | 0.74 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD12 | 2 | 0.74 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD12 | 18 | 0.74 |
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 18 | 0.73 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 7 | 0.73 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 4 | 0.73 |
| (2,1167) | 1:47:A:ILE:HG22 | 1:20:A:ASP:H | 1 | 0.73 |
| (2,1167) | 1:47:A:ILE:HG22 | 1:20:A:ASP:H | 5 | 0.73 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 16 | 0.73 |
| (2,892) | 1:69:A:THR:HG22 | 1:19:A:CYS:HA | 7 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 9 | 0.73 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD13 | 1 | 0.73 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD12 | 14 | 0.73 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD12 | 15 | 0.73 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 1 | 0.72 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 16 | 0.72 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 13 | 0.72 |
| (2,1181) | 1:79:A:LEU:HD22 | 1:51:A:GLN:H | 14 | 0.72 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 19 | 0.72 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 17 | 0.72 |
| (2,1102) | 1:48:A:GLN:H | 1:23:A:LYS:HB2 | 20 | 0.72 |
| (2,1090) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HE22 | 5 | 0.72 |
| (2,1090) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE22 | 10 | 0.72 |
| (2,863) | 1:41:A:VAL:HG13 | 1:40:A:ASP:HB2 | 4 | 0.72 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 12 | 0.72 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG21 | 4 | 0.72 |
| (2,415) | 1:45:A:VAL:HG13 | 1:45:A:VAL:HA | 8 | 0.72 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 19 | 0.72 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 17 | 0.72 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD12 | 9 | 0.72 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD12 | 10 | 0.72 |
| (2,50) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HD13 | 19 | 0.72 |
| (2,1253) | 1:16:A:LEU:HD13 | 1:4:A:TRP:HE1 | 12 | 0.71 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 9 | 0.71 |
| (2,1131) | 1:23:A:LYS:HG3 | 1:22:A:ASN:H | 9 | 0.71 |
| (2,892) | 1:69:A:THR:HG22 | 1:19:A:CYS:HA | 6 | 0.71 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 10 | 0.71 |
| (2,630) | 1:52:A:ILE:HD12 | 1:64:A:CYS:HB3 | 15 | 0.71 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 12 | 0.71 |
| (2,415) | 1:45:A:VAL:HG11 | 1:45:A:VAL:HA | 13 | 0.71 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 4 | 0.71 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 17 | 0.71 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 13 | 0.71 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 9 | 0.71 |
| (2,1253) | 1:16:A:LEU:HD13 | 1:4:A:TRP:HE1 | 2 | 0.7 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 9 | 0.7 |
| (2,1210) | 1:46:A:ALA:HB3 | 1:26:A:GLN:H | 8 | 0.7 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 13 | 0.7 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 19 | 0.7 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 14 | 0.7 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 18 | 0.7 |
| (2,1167) | 1:47:A:ILE:HG22 | 1:20:A:ASP:H | 4 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,906) | 1:7:A:LYS:HG3 | 1:8:A:THR:HA | 4 | 0.7 |
| (2,892) | 1:69:A:THR:HG22 | 1:19:A:CYS:HA | 15 | 0.7 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 6 | 0.7 |
| (2,536) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HA | 20 | 0.7 |
| (2,504) | 1:7:A:LYS:HD3 | 1:7:A:LYS:HA | 19 | 0.7 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 13 | 0.7 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 9 | 0.7 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD13 | 4 | 0.7 |
| (2,50) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HD12 | 6 | 0.7 |
| (2,50) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HD12 | 7 | 0.7 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 13 | 0.69 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 4 | 0.69 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 6 | 0.69 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 10 | 0.69 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 15 | 0.69 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 3 | 0.69 |
| (2,1158) | 1:45:A:VAL:HG22 | 1:46:A:ALA:H | 18 | 0.69 |
| (2,948) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE21 | 6 | 0.69 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 20 | 0.69 |
| (2,805) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HG3 | 17 | 0.69 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 13 | 0.69 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 6 | 0.69 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB2 | 7 | 0.69 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 1 | 0.69 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 15 | 0.69 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 2 | 0.69 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 6 | 0.69 |
| (2,1253) | 1:16:A:LEU:HD12 | 1:4:A:TRP:HE1 | 17 | 0.68 |
| (2,1213) | 1:45:A:VAL:HG23 | 1:83:A:ASN:H | 15 | 0.68 |
| (2,1210) | 1:46:A:ALA:HB3 | 1:26:A:GLN:H | 17 | 0.68 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 11 | 0.68 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 15 | 0.68 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 19 | 0.68 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 20 | 0.68 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 16 | 0.68 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 2 | 0.68 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 9 | 0.68 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 10 | 0.68 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 12 | 0.68 |
| (2,1158) | 1:45:A:VAL:HG22 | 1:46:A:ALA:H | 6 | 0.68 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 4 | 0.68 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG23 | 19 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG23 | 6 | 0.68 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 13 | 0.68 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 9 | 0.68 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 20 | 0.68 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 11 | 0.68 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 20 | 0.68 |
| (2,504) | 1:7:A:LYS:HD3 | 1:7:A:LYS:HA | 3 | 0.68 |
| (2,415) | 1:45:A:VAL:HG13 | 1:45:A:VAL:HA | 4 | 0.68 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG23 | 14 | 0.68 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG23 | 15 | 0.68 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 6 | 0.68 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 3 | 0.68 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 1 | 0.67 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 5 | 0.67 |
| (2,1223) | 1:27:A:LYS:HE3 | 1:27:A:LYS:H | 4 | 0.67 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 10 | 0.67 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 3 | 0.67 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 8 | 0.67 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 11 | 0.67 |
| (2,1167) | 1:47:A:ILE:HG22 | 1:20:A:ASP:H | 18 | 0.67 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 15 | 0.67 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 9 | 0.67 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD21 | 17 | 0.67 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 18 | 0.67 |
| (2,504) | 1:7:A:LYS:HD3 | 1:7:A:LYS:HA | 13 | 0.67 |
| (2,415) | 1:45:A:VAL:HG13 | 1:45:A:VAL:HA | 10 | 0.67 |
| (2,415) | 1:45:A:VAL:HG11 | 1:45:A:VAL:HA | 11 | 0.67 |
| (2,313) | 1:52:A:ILE:HB | 1:52:A:ILE:HD13 | 15 | 0.67 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG21 | 19 | 0.67 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 16 | 0.67 |
| (2,159) | 1:56:A:ILE:HB | 1:56:A:ILE:HD13 | 14 | 0.67 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 11 | 0.67 |
| (2,40) | 1:46:A:ALA:HB1 | 1:45:A:VAL:HA | 18 | 0.67 |
| (2,1253) | 1:16:A:LEU:HD12 | 1:4:A:TRP:HE1 | 20 | 0.66 |
| (2,1223) | 1:27:A:LYS:HE3 | 1:27:A:LYS:H | 7 | 0.66 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 13 | 0.66 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 12 | 0.66 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 18 | 0.66 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 3 | 0.66 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 6 | 0.66 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 7 | 0.66 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 19 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 7 | 0.66 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 20 | 0.66 |
| (2,965) | 1:42:A:LEU:HB3 | 1:42:A:LEU:H | 10 | 0.66 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 12 | 0.66 |
| (2,863) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB2 | 2 | 0.66 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 7 | 0.66 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD22 | 11 | 0.66 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG23 | 2 | 0.66 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB2 | 20 | 0.66 |
| (2,536) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HA | 1 | 0.66 |
| (2,428) | 1:59:A:ALA:HB1 | 1:62:A:ASP:HB3 | 16 | 0.66 |
| (2,415) | 1:45:A:VAL:HG12 | 1:45:A:VAL:HA | 20 | 0.66 |
| (2,323) | 1:69:A:THR:HG21 | 1:86:A:PRO:HD2 | 2 | 0.66 |
| (2,313) | 1:52:A:ILE:HB | 1:52:A:ILE:HD13 | 19 | 0.66 |
| (2,205) | 1:74:A:VAL:HG21 | 1:15:A:LYS:HE3 | 9 | 0.66 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 8 | 0.66 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 7 | 0.65 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 9 | 0.65 |
| (2,1158) | 1:45:A:VAL:HG22 | 1:46:A:ALA:H | 12 | 0.65 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 18 | 0.65 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 11 | 0.65 |
| (2,892) | 1:69:A:THR:HG23 | 1:19:A:CYS:HA | 19 | 0.65 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 14 | 0.65 |
| (2,805) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HG3 | 2 | 0.65 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 7 | 0.65 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 3 | 0.65 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 15 | 0.65 |
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 18 | 0.65 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG22 | 14 | 0.65 |
| (2,451) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB2 | 10 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 1 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 4 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 8 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 9 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 12 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 13 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 14 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 16 | 0.65 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 20 | 0.65 |
| (2,205) | 1:74:A:VAL:HG23 | 1:15:A:LYS:HE3 | 1 | 0.65 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 14 | 0.65 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 17 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 14 | 0.65 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 9 | 0.65 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 7 | 0.65 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 12 | 0.65 |
| (2,1253) | 1:16:A:LEU:HD12 | 1:4:A:TRP:HE1 | 6 | 0.64 |
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 1 | 0.64 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 5 | 0.64 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 14 | 0.64 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 20 | 0.64 |
| (2,1181) | 1:79:A:LEU:HD22 | 1:51:A:GLN:H | 6 | 0.64 |
| (2,1158) | 1:45:A:VAL:HG23 | 1:46:A:ALA:H | 17 | 0.64 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 1 | 0.64 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 13 | 0.64 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG22 | 16 | 0.64 |
| (2,892) | 1:69:A:THR:HG22 | 1:19:A:CYS:HA | 2 | 0.64 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 4 | 0.64 |
| (2,892) | 1:69:A:THR:HG22 | 1:19:A:CYS:HA | 18 | 0.64 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 14 | 0.64 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 13 | 0.64 |
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 4 | 0.64 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG23 | 20 | 0.64 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 15 | 0.64 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 17 | 0.64 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 6 | 0.64 |
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 6 | 0.64 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 4 | 0.64 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 10 | 0.64 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 12 | 0.64 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 16 | 0.64 |
| (2,62) | 1:50:A:THR:HG22 | 1:50:A:THR:HA | 19 | 0.64 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 14 | 0.64 |
| (2,1253) | 1:16:A:LEU:HD13 | 1:4:A:TRP:HE1 | 16 | 0.63 |
| (2,1197) | 1:35:A:LEU:H | 1:35:A:LEU:HB3 | 2 | 0.63 |
| (2,1191) | 1:54:A:LEU:HB2 | 1:54:A:LEU:H | 1 | 0.63 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 1 | 0.63 |
| (2,892) | 1:69:A:THR:HG23 | 1:19:A:CYS:HA | 9 | 0.63 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 10 | 0.63 |
| (2,863) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB2 | 7 | 0.63 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 16 | 0.63 |
| (2,615) | 1:46:A:ALA:HB2 | 1:25:A:VAL:HG22 | 17 | 0.63 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG23 | 19 | 0.63 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 6 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD12 | 8 | 0.63 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 9 | 0.63 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 4 | 0.63 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 5 | 0.63 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 12 | 0.63 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 2 | 0.63 |
| (2,62) | 1:50:A:THR:HG22 | 1:50:A:THR:HA | 3 | 0.63 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 9 | 0.63 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 15 | 0.63 |
| (2,62) | 1:50:A:THR:HG22 | 1:50:A:THR:HA | 18 | 0.63 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 20 | 0.63 |
| (1,24) | 1:41:A:VAL:HG11 | 1:42:A:LEU:H | 9 | 0.63 |
| (1,24) | 1:41:A:VAL:HG21 | 1:42:A:LEU:H | 15 | 0.63 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 8 | 0.62 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 6 | 0.62 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 16 | 0.62 |
| (2,948) | 1:80:A:VAL:HG11 | 1:48:A:GLN:HE21 | 12 | 0.62 |
| (2,892) | 1:69:A:THR:HG23 | 1:19:A:CYS:HA | 3 | 0.62 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 15 | 0.62 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 12 | 0.62 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 17 | 0.62 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 1 | 0.62 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 14 | 0.62 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 14 | 0.62 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 2 | 0.62 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 20 | 0.62 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 11 | 0.62 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 1 | 0.62 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 4 | 0.62 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD12 | 13 | 0.62 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 14 | 0.62 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD12 | 16 | 0.62 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 6 | 0.62 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 15 | 0.62 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 10 | 0.62 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 5 | 0.62 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 7 | 0.62 |
| (2,62) | 1:50:A:THR:HG22 | 1:50:A:THR:HA | 11 | 0.62 |
| (2,62) | 1:50:A:THR:HG22 | 1:50:A:THR:HA | 14 | 0.62 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 10 | 0.62 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 17 | 0.62 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 18 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 14 | 0.61 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 8 | 0.61 |
| (2,1210) | 1:46:A:ALA:HB2 | 1:26:A:GLN:H | 12 | 0.61 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 7 | 0.61 |
| (2,1143) | 1:25:A:VAL:HG23 | 1:24:A:LYS:H | 15 | 0.61 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 8 | 0.61 |
| (2,1086) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 16 | 0.61 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 5 | 0.61 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 14 | 0.61 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 3 | 0.61 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 13 | 0.61 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 1 | 0.61 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 20 | 0.61 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 18 | 0.61 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 1 | 0.61 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 15 | 0.61 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 4 | 0.61 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 14 | 0.61 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG21 | 7 | 0.61 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG23 | 9 | 0.61 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 4 | 0.61 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 11 | 0.61 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 17 | 0.61 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 18 | 0.61 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 10 | 0.61 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 15 | 0.61 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 20 | 0.61 |
| (2,147) | 1:24:A:LYS:H | 1:24:A:LYS:HB2 | 1 | 0.61 |
| (2,147) | 1:24:A:LYS:H | 1:24:A:LYS:HB2 | 4 | 0.61 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 7 | 0.61 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 17 | 0.61 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 6 | 0.61 |
| (2,40) | 1:46:A:ALA:HB1 | 1:45:A:VAL:HA | 3 | 0.61 |
| (2,40) | 1:46:A:ALA:HB1 | 1:45:A:VAL:HA | 5 | 0.61 |
| (2,1255) | 1:82:A:ILE:HD11 | 1:44:A:GLN:HE21 | 2 | 0.6 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 2 | 0.6 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 4 | 0.6 |
| (2,1167) | 1:47:A:ILE:HG23 | 1:20:A:ASP:H | 20 | 0.6 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 19 | 0.6 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 1 | 0.6 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 10 | 0.6 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 1 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 2 | 0.6 |
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 13 | 0.6 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 7 | 0.6 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 14 | 0.6 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 6 | 0.6 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 7 | 0.6 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 6 | 0.6 |
| (2,615) | 1:46:A:ALA:HB2 | 1:25:A:VAL:HG22 | 8 | 0.6 |
| (2,615) | 1:46:A:ALA:HB2 | 1:25:A:VAL:HG21 | 9 | 0.6 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 18 | 0.6 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 2 | 0.6 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 9 | 0.6 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD12 | 18 | 0.6 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 15 | 0.6 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG21 | 15 | 0.6 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 5 | 0.6 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 7 | 0.6 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 13 | 0.6 |
| (2,206) | 1:73:A:ASP:HA | 1:15:A:LYS:HE2 | 11 | 0.6 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 1 | 0.6 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 11 | 0.6 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 1 | 0.6 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 13 | 0.6 |
| (2,1167) | 1:47:A:ILE:HG21 | 1:20:A:ASP:H | 14 | 0.59 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 20 | 0.59 |
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 9 | 0.59 |
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 10 | 0.59 |
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 14 | 0.59 |
| (2,1046) | 1:13:A:THR:HG21 | 1:12:A:ASN:HD22 | 11 | 0.59 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 1 | 0.59 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 11 | 0.59 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD21 | 1 | 0.59 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG22 | 7 | 0.59 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 19 | 0.59 |
| (2,323) | 1:69:A:THR:HG21 | 1:86:A:PRO:HD2 | 18 | 0.59 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 3 | 0.59 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 14 | 0.59 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG23 | 6 | 0.59 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 1 | 0.59 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 3 | 0.59 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 16 | 0.59 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 14 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 9 | 0.59 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 14 | 0.59 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 1 | 0.59 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 9 | 0.59 |
| (2,40) | 1:46:A:ALA:HB1 | 1:45:A:VAL:HA | 4 | 0.59 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 20 | 0.59 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 1 | 0.59 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 19 | 0.59 |
| (2,1181) | 1:79:A:LEU:HD21 | 1:51:A:GLN:H | 8 | 0.58 |
| (2,1143) | 1:25:A:VAL:HG23 | 1:24:A:LYS:H | 14 | 0.58 |
| (2,1124) | 1:41:A:VAL:HG23 | 1:44:A:GLN:HE22 | 15 | 0.58 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 7 | 0.58 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 5 | 0.58 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 10 | 0.58 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 9 | 0.58 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 13 | 0.58 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 18 | 0.58 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD22 | 4 | 0.58 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD23 | 8 | 0.58 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD22 | 14 | 0.58 |
| (2,768) | 1:22:A:ASN:H | 1:22:A:ASN:HB2 | 13 | 0.58 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 15 | 0.58 |
| (2,670) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HG2 | 2 | 0.58 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 5 | 0.58 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 10 | 0.58 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 19 | 0.58 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 15 | 0.58 |
| (2,452) | 1:72:A:GLU:H | 1:72:A:GLU:HB3 | 6 | 0.58 |
| (2,452) | 1:72:A:GLU:H | 1:72:A:GLU:HB3 | 10 | 0.58 |
| (2,451) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB2 | 6 | 0.58 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 16 | 0.58 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 12 | 0.58 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 7 | 0.58 |
| (2,292) | 1:16:A:LEU:HD12 | 1:16:A:LEU:HB3 | 17 | 0.58 |
| (2,292) | 1:16:A:LEU:HD12 | 1:16:A:LEU:HB3 | 20 | 0.58 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG22 | 3 | 0.58 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG22 | 20 | 0.58 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 1 | 0.58 |
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 17 | 0.58 |
| (2,1253) | 1:16:A:LEU:HD13 | 1:4:A:TRP:HE1 | 18 | 0.57 |
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 4 | 0.57 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 5 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG22 | 11 | 0.57 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 3 | 0.57 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 5 | 0.57 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD22 | 20 | 0.57 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG23 | 2 | 0.57 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 12 | 0.57 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 18 | 0.57 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 4 | 0.57 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 12 | 0.57 |
| (2,452) | 1:72:A:GLU:H | 1:72:A:GLU:HB3 | 9 | 0.57 |
| (2,452) | 1:72:A:GLU:H | 1:72:A:GLU:HB3 | 18 | 0.57 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 3 | 0.57 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 4 | 0.57 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 19 | 0.57 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 4 | 0.57 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 10 | 0.57 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 5 | 0.57 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 10 | 0.57 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 11 | 0.57 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 1 | 0.57 |
| (2,292) | 1:16:A:LEU:HD12 | 1:16:A:LEU:HB3 | 3 | 0.57 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 4 | 0.57 |
| (2,292) | 1:16:A:LEU:HD12 | 1:16:A:LEU:HB3 | 6 | 0.57 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 13 | 0.57 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 19 | 0.57 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG21 | 18 | 0.57 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 13 | 0.57 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 1 | 0.57 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 12 | 0.57 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 8 | 0.57 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 15 | 0.57 |
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 2 | 0.57 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 11 | 0.57 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 16 | 0.57 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 8 | 0.57 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 1 | 0.56 |
| (2,1255) | 1:82:A:ILE:HD11 | 1:44:A:GLN:HE21 | 8 | 0.56 |
| (2,1255) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE21 | 12 | 0.56 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 1 | 0.56 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 16 | 0.56 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 7 | 0.56 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 10 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 5 | 0.56 |
| (2,1086) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 20 | 0.56 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 6 | 0.56 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG22 | 4 | 0.56 |
| (2,892) | 1:69:A:THR:HG23 | 1:19:A:CYS:HA | 16 | 0.56 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 20 | 0.56 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 13 | 0.56 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG23 | 3 | 0.56 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD22 | 6 | 0.56 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD22 | 10 | 0.56 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 2 | 0.56 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 9 | 0.56 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 2 | 0.56 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG22 | 10 | 0.56 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 8 | 0.56 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 9 | 0.56 |
| (2,502) | 1:58:A:ILE:HG21 | 1:63:A:GLU:HG3 | 20 | 0.56 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 6 | 0.56 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 8 | 0.56 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 9 | 0.56 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 20 | 0.56 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 5 | 0.56 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 10 | 0.56 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG23 | 2 | 0.56 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 2 | 0.56 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 14 | 0.56 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 17 | 0.56 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 1 | 0.56 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 13 | 0.56 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 18 | 0.56 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 8 | 0.56 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 9 | 0.56 |
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 13 | 0.56 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 19 | 0.56 |
| (2,62) | 1:50:A:THR:HG21 | 1:50:A:THR:HA | 8 | 0.56 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 19 | 0.56 |
| (2,1158) | 1:45:A:VAL:HG23 | 1:46:A:ALA:H | 5 | 0.55 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 9 | 0.55 |
| (2,1086) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 11 | 0.55 |
| (2,1086) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 12 | 0.55 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 17 | 0.55 |
| (2,1072) | 1:31:A:GLU:H | 1:31:A:GLU:HG2 | 9 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1046) | 1:13:A:THR:HG22 | 1:12:A:ASN:HD22 | 4 | 0.55 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 9 | 0.55 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG22 | 7 | 0.55 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 8 | 0.55 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 5 | 0.55 |
| (2,892) | 1:69:A:THR:HG21 | 1:19:A:CYS:HA | 8 | 0.55 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 8 | 0.55 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 9 | 0.55 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 6 | 0.55 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD22 | 1 | 0.55 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 1 | 0.55 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 3 | 0.55 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG22 | 16 | 0.55 |
| (2,600) | 1:47:A:ILE:HD13 | 1:21:A:THR:HB | 16 | 0.55 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB2 | 5 | 0.55 |
| (2,453) | 1:73:A:ASP:H | 1:72:A:GLU:HB3 | 10 | 0.55 |
| (2,451) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB2 | 9 | 0.55 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 2 | 0.55 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 13 | 0.55 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 16 | 0.55 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 12 | 0.55 |
| (2,292) | 1:16:A:LEU:HD12 | 1:16:A:LEU:HB3 | 7 | 0.55 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 9 | 0.55 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 11 | 0.55 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG21 | 12 | 0.55 |
| (2,225) | 1:54:A:LEU:HD22 | 1:54:A:LEU:HA | 10 | 0.55 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 11 | 0.55 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 18 | 0.55 |
| (2,40) | 1:46:A:ALA:HB3 | 1:45:A:VAL:HA | 13 | 0.55 |
| (1,30) | 1:35:A:LEU:HD23 | 1:36:A:LEU:H | 11 | 0.55 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 18 | 0.54 |
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 19 | 0.54 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 10 | 0.54 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 11 | 0.54 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 13 | 0.54 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 14 | 0.54 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 19 | 0.54 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 12 | 0.54 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 18 | 0.54 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 16 | 0.54 |
| (2,906) | 1:7:A:LYS:HG3 | 1:8:A:THR:HA | 11 | 0.54 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 3 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG22 | 14 | 0.54 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 17 | 0.54 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 9 | 0.54 |
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 13 | 0.54 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 6 | 0.54 |
| (2,502) | 1:58:A:ILE:HG23 | 1:63:A:GLU:HG3 | 10 | 0.54 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG23 | 8 | 0.54 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 1 | 0.54 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 17 | 0.54 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 20 | 0.54 |
| (2,292) | 1:16:A:LEU:HD13 | 1:16:A:LEU:HB3 | 2 | 0.54 |
| (2,292) | 1:16:A:LEU:HD11 | 1:16:A:LEU:HB3 | 8 | 0.54 |
| (2,292) | 1:16:A:LEU:HD13 | 1:16:A:LEU:HB3 | 18 | 0.54 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 9 | 0.54 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG21 | 10 | 0.54 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG21 | 13 | 0.54 |
| (2,225) | 1:54:A:LEU:HD23 | 1:54:A:LEU:HA | 1 | 0.54 |
| (2,225) | 1:54:A:LEU:HD21 | 1:54:A:LEU:HA | 18 | 0.54 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 20 | 0.54 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 12 | 0.54 |
| (2,40) | 1:46:A:ALA:HB1 | 1:45:A:VAL:HA | 1 | 0.54 |
| (2,40) | 1:46:A:ALA:HB2 | 1:45:A:VAL:HA | 15 | 0.54 |
| (1,24) | 1:41:A:VAL:HG11 | 1:42:A:LEU:H | 13 | 0.54 |
| (2,1213) | 1:45:A:VAL:HG22 | 1:83:A:ASN:H | 5 | 0.53 |
| (2,1210) | 1:46:A:ALA:HB2 | 1:26:A:GLN:H | 14 | 0.53 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 11 | 0.53 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 12 | 0.53 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 9 | 0.53 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 16 | 0.53 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 17 | 0.53 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG21 | 12 | 0.53 |
| (2,940) | 1:79:A:LEU:HD21 | 1:49:A:CYS:H | 17 | 0.53 |
| (2,907) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HG3 | 17 | 0.53 |
| (2,873) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HG3 | 5 | 0.53 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 1 | 0.53 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 18 | 0.53 |
| (2,661) | 1:74:A:VAL:HG11 | 1:78:A:GLY:HA3 | 8 | 0.53 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG21 | 11 | 0.53 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG21 | 12 | 0.53 |
| (2,502) | 1:58:A:ILE:HG23 | 1:63:A:GLU:HG3 | 3 | 0.53 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 8 | 0.53 |
| (2,292) | 1:16:A:LEU:HD13 | 1:16:A:LEU:HB3 | 12 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,292) | 1:16:A:LEU:HD13 | 1:16:A:LEU:HB3 | 16 | 0.53 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG22 | 8 | 0.53 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG23 | 16 | 0.53 |
| (2,225) | 1:54:A:LEU:HD21 | 1:54:A:LEU:HA | 4 | 0.53 |
| (2,225) | 1:54:A:LEU:HD21 | 1:54:A:LEU:HA | 5 | 0.53 |
| (2,225) | 1:54:A:LEU:HD21 | 1:54:A:LEU:HA | 12 | 0.53 |
| (2,225) | 1:54:A:LEU:HD23 | 1:54:A:LEU:HA | 14 | 0.53 |
| (2,225) | 1:54:A:LEU:HD22 | 1:54:A:LEU:HA | 16 | 0.53 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 5 | 0.53 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 18 | 0.53 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 1 | 0.53 |
| (2,95) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HA | 3 | 0.53 |
| (2,62) | 1:50:A:THR:HG23 | 1:50:A:THR:HA | 17 | 0.53 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 3 | 0.53 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD12 | 9 | 0.53 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD11 | 12 | 0.53 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD11 | 16 | 0.53 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 18 | 0.53 |
| (1,30) | 1:35:A:LEU:HD21 | 1:36:A:LEU:H | 9 | 0.53 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 16 | 0.53 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 8 | 0.52 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 13 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 2 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 3 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 6 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 7 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 8 | 0.52 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 15 | 0.52 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 1 | 0.52 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 11 | 0.52 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 13 | 0.52 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 14 | 0.52 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG21 | 5 | 0.52 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG23 | 13 | 0.52 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 20 | 0.52 |
| (2,825) | 1:8:A:THR:HG22 | 1:10:A:SER:HB3 | 18 | 0.52 |
| (2,600) | 1:47:A:ILE:HD13 | 1:21:A:THR:HB | 10 | 0.52 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 6 | 0.52 |
| (2,502) | 1:58:A:ILE:HG21 | 1:63:A:GLU:HG3 | 8 | 0.52 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 18 | 0.52 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 14 | 0.52 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 5 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 2 | 0.52 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG23 | 1 | 0.52 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG23 | 2 | 0.52 |
| (2,225) | 1:54:A:LEU:HD23 | 1:54:A:LEU:HA | 7 | 0.52 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 8 | 0.52 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 9 | 0.52 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 15 | 0.52 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 7 | 0.52 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 16 | 0.52 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 15 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD11 | 1 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD11 | 4 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD12 | 5 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 6 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 7 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 10 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 11 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD12 | 13 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD12 | 14 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 15 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 17 | 0.52 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD12 | 20 | 0.52 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 5 | 0.52 |
| (1,24) | 1:41:A:VAL:HG11 | 1:42:A:LEU:H | 14 | 0.52 |
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 5 | 0.51 |
| (2,1213) | 1:45:A:VAL:HG23 | 1:83:A:ASN:H | 7 | 0.51 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 5 | 0.51 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 16 | 0.51 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 1 | 0.51 |
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 8 | 0.51 |
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 9 | 0.51 |
| (2,1086) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 15 | 0.51 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 10 | 0.51 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 15 | 0.51 |
| (2,997) | 1:60:A:ILE:HD13 | 1:69:A:THR:H | 9 | 0.51 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 1 | 0.51 |
| (2,860) | 1:36:A:LEU:HA | 1:36:A:LEU:HD23 | 16 | 0.51 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 7 | 0.51 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 6 | 0.51 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 17 | 0.51 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 7 | 0.51 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 13 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 3 | 0.51 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 7 | 0.51 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 9 | 0.51 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 11 | 0.51 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 18 | 0.51 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 11 | 0.51 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 12 | 0.51 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 16 | 0.51 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 17 | 0.51 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 20 | 0.51 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 7 | 0.51 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 11 | 0.51 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 12 | 0.51 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG21 | 17 | 0.51 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG21 | 8 | 0.51 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 11 | 0.51 |
| (2,180) | 1:69:A:THR:HG21 | 1:86:A:PRO:HB2 | 7 | 0.51 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 17 | 0.51 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 2 | 0.51 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 6 | 0.51 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 7 | 0.51 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 2 | 0.51 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 4 | 0.51 |
| (2,95) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HA | 16 | 0.51 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 2 | 0.51 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 8 | 0.51 |
| (1,30) | 1:35:A:LEU:HD23 | 1:36:A:LEU:H | 16 | 0.51 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 3 | 0.51 |
| (1,24) | 1:41:A:VAL:HG11 | 1:42:A:LEU:H | 4 | 0.51 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 11 | 0.5 |
| (2,1223) | 1:27:A:LYS:HE3 | 1:27:A:LYS:H | 5 | 0.5 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 18 | 0.5 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 16 | 0.5 |
| (2,1158) | 1:45:A:VAL:HG21 | 1:46:A:ALA:H | 15 | 0.5 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 7 | 0.5 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 12 | 0.5 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 4 | 0.5 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 5 | 0.5 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 18 | 0.5 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 20 | 0.5 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 4 | 0.5 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 19 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,972) | 1:23:A:LYS:H | 1:23:A:LYS:HG3 | 9 | 0.5 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG22 | 1 | 0.5 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG21 | 4 | 0.5 |
| (2,940) | 1:79:A:LEU:HD23 | 1:49:A:CYS:H | 5 | 0.5 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 5 | 0.5 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD11 | 10 | 0.5 |
| (2,815) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB3 | 5 | 0.5 |
| (2,790) | 1:60:A:ILE:HD13 | 1:68:A:PRO:HA | 13 | 0.5 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD12 | 12 | 0.5 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 14 | 0.5 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 17 | 0.5 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG21 | 14 | 0.5 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 3 | 0.5 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 13 | 0.5 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 19 | 0.5 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 5 | 0.5 |
| (2,646) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 2 | 0.5 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 17 | 0.5 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 19 | 0.5 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 7 | 0.5 |
| (2,502) | 1:58:A:ILE:HG23 | 1:63:A:GLU:HG3 | 7 | 0.5 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 15 | 0.5 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 16 | 0.5 |
| (2,453) | 1:73:A:ASP:H | 1:72:A:GLU:HB3 | 6 | 0.5 |
| (2,428) | 1:59:A:ALA:HB3 | 1:62:A:ASP:HB3 | 7 | 0.5 |
| (2,398) | 1:2:A:SER:HB3 | 1:2:A:SER:HA | 7 | 0.5 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 20 | 0.5 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 3 | 0.5 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 10 | 0.5 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 15 | 0.5 |
| (2,318) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB2 | 18 | 0.5 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD13 | 17 | 0.5 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG22 | 19 | 0.5 |
| (2,225) | 1:54:A:LEU:HD22 | 1:54:A:LEU:HA | 13 | 0.5 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG22 | 9 | 0.5 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 8 | 0.5 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 20 | 0.5 |
| (2,95) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HA | 20 | 0.5 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 12 | 0.5 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 14 | 0.49 |
| (2,1221) | 1:27:A:LYS:H | 1:27:A:LYS:HB2 | 6 | 0.49 |
| (2,1210) | 1:46:A:ALA:HB3 | 1:26:A:GLN:H | 3 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 7 | 0.49 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 5 | 0.49 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 17 | 0.49 |
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 12 | 0.49 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 5 | 0.49 |
| (2,1086) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 18 | 0.49 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 20 | 0.49 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 12 | 0.49 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 3 | 0.49 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 8 | 0.49 |
| (2,997) | 1:60:A:ILE:HD11 | 1:69:A:THR:H | 20 | 0.49 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 12 | 0.49 |
| (2,863) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB2 | 16 | 0.49 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 11 | 0.49 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 20 | 0.49 |
| (2,773) | 1:79:A:LEU:HB3 | 1:79:A:LEU:HD23 | 9 | 0.49 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 20 | 0.49 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 2 | 0.49 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 7 | 0.49 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 4 | 0.49 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 15 | 0.49 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 17 | 0.49 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG22 | 1 | 0.49 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 7 | 0.49 |
| (2,615) | 1:46:A:ALA:HB1 | 1:25:A:VAL:HG22 | 13 | 0.49 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG21 | 15 | 0.49 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 8 | 0.49 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 19 | 0.49 |
| (2,428) | 1:59:A:ALA:HB3 | 1:62:A:ASP:HB3 | 5 | 0.49 |
| (2,323) | 1:69:A:THR:HG21 | 1:86:A:PRO:HD2 | 6 | 0.49 |
| (2,323) | 1:69:A:THR:HG21 | 1:86:A:PRO:HD2 | 7 | 0.49 |
| (2,312) | 1:52:A:ILE:HA | 1:52:A:ILE:HD11 | 6 | 0.49 |
| (2,308) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HD11 | 5 | 0.49 |
| (2,247) | 1:59:A:ALA:HB3 | 1:58:A:ILE:HG23 | 5 | 0.49 |
| (2,227) | 1:88:A:PRO:HA | 1:88:A:PRO:HG3 | 12 | 0.49 |
| (2,225) | 1:54:A:LEU:HD22 | 1:54:A:LEU:HA | 9 | 0.49 |
| (2,225) | 1:54:A:LEU:HD23 | 1:54:A:LEU:HA | 20 | 0.49 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 13 | 0.49 |
| (2,49) | 1:58:A:ILE:HB | 1:58:A:ILE:HD13 | 19 | 0.49 |
| (1,30) | 1:35:A:LEU:HD23 | 1:36:A:LEU:H | 14 | 0.49 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 14 | 0.48 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 2 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1086) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 3 | 0.48 |
| (2,1021) | 1:44:A:GLN:H | 1:44:A:GLN:HB3 | 1 | 0.48 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 2 | 0.48 |
| (2,997) | 1:60:A:ILE:HD12 | 1:69:A:THR:H | 16 | 0.48 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG22 | 10 | 0.48 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG22 | 12 | 0.48 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 17 | 0.48 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 12 | 0.48 |
| (2,906) | 1:7:A:LYS:HG3 | 1:8:A:THR:HA | 15 | 0.48 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 6 | 0.48 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 8 | 0.48 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 9 | 0.48 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 9 | 0.48 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 8 | 0.48 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 16 | 0.48 |
| (2,711) | 1:25:A:VAL:HG22 | 1:48:A:GLN:HG2 | 5 | 0.48 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 10 | 0.48 |
| (2,600) | 1:47:A:ILE:HD11 | 1:21:A:THR:HB | 2 | 0.48 |
| (2,577) | 1:16:A:LEU:HD13 | 1:11:A:CYS:HB3 | 5 | 0.48 |
| (2,541) | 1:87:A:ILE:HG23 | 1:10:A:SER:HA | 12 | 0.48 |
| (2,541) | 1:87:A:ILE:HG21 | 1:10:A:SER:HA | 16 | 0.48 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 1 | 0.48 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 4 | 0.48 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 5 | 0.48 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 20 | 0.48 |
| (2,428) | 1:59:A:ALA:HB1 | 1:62:A:ASP:HB3 | 13 | 0.48 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 10 | 0.48 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 8 | 0.48 |
| (2,151) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HA | 6 | 0.48 |
| (2,151) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HA | 10 | 0.48 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 19 | 0.48 |
| (1,24) | 1:41:A:VAL:HG11 | 1:42:A:LEU:H | 17 | 0.48 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 4 | 0.47 |
| (2,1158) | 1:45:A:VAL:HG22 | 1:46:A:ALA:H | 1 | 0.47 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 17 | 0.47 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 10 | 0.47 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 20 | 0.47 |
| (2,961) | 1:8:A:THR:H | 1:8:A:THR:HG21 | 10 | 0.47 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 6 | 0.47 |
| (2,863) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB2 | 5 | 0.47 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 8 | 0.47 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 10 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 13 | 0.47 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 12 | 0.47 |
| (2,722) | 1:87:A:ILE:HG23 | 1:70:A:CYS:HB3 | 5 | 0.47 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 3 | 0.47 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 20 | 0.47 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 20 | 0.47 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 1 | 0.47 |
| (2,600) | 1:47:A:ILE:HD13 | 1:21:A:THR:HB | 13 | 0.47 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 17 | 0.47 |
| (2,543) | 1:79:A:LEU:HD21 | 1:50:A:THR:HA | 17 | 0.47 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 1 | 0.47 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 19 | 0.47 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 5 | 0.47 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 10 | 0.47 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG21 | 13 | 0.47 |
| (2,451) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB2 | 18 | 0.47 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 5 | 0.47 |
| (2,334) | 1:51:A:GLN:HG3 | 1:51:A:GLN:HA | 17 | 0.47 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 11 | 0.47 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 20 | 0.47 |
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 9 | 0.47 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 3 | 0.47 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 4 | 0.47 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG21 | 16 | 0.47 |
| (2,151) | 1:60:A:ILE:HD12 | 1:60:A:ILE:HA | 12 | 0.47 |
| (2,151) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HA | 17 | 0.47 |
| (2,147) | 1:24:A:LYS:H | 1:24:A:LYS:HB2 | 12 | 0.47 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD11 | 5 | 0.47 |
| (1,30) | 1:35:A:LEU:HD23 | 1:36:A:LEU:H | 4 | 0.47 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 11 | 0.47 |
| (2,1223) | 1:27:A:LYS:HE3 | 1:27:A:LYS:H | 15 | 0.46 |
| (2,1208) | 1:26:A:GLN:H | 1:26:A:GLN:HB2 | 13 | 0.46 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 3 | 0.46 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 16 | 0.46 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 18 | 0.46 |
| (2,1031) | 1:10:A:SER:H | 1:10:A:SER:HB3 | 1 | 0.46 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 2 | 0.46 |
| (2,907) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HG3 | 1 | 0.46 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 7 | 0.46 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 15 | 0.46 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 17 | 0.46 |
| (2,828) | 1:60:A:ILE:HD13 | 1:64:A:CYS:HB3 | 12 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 8 | 0.46 |
| (2,815) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB3 | 15 | 0.46 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD12 | 7 | 0.46 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 15 | 0.46 |
| (2,722) | 1:87:A:ILE:HG22 | 1:70:A:CYS:HB3 | 6 | 0.46 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 3 | 0.46 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG23 | 4 | 0.46 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 12 | 0.46 |
| (2,600) | 1:47:A:ILE:HD11 | 1:21:A:THR:HB | 3 | 0.46 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 11 | 0.46 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 2 | 0.46 |
| (2,502) | 1:58:A:ILE:HG23 | 1:63:A:GLU:HG3 | 18 | 0.46 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 6 | 0.46 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG23 | 3 | 0.46 |
| (2,453) | 1:73:A:ASP:H | 1:72:A:GLU:HB3 | 9 | 0.46 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 10 | 0.46 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 6 | 0.46 |
| (2,247) | 1:59:A:ALA:HB2 | 1:58:A:ILE:HG23 | 4 | 0.46 |
| (2,180) | 1:69:A:THR:HG21 | 1:86:A:PRO:HB2 | 2 | 0.46 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 3 | 0.46 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG22 | 7 | 0.46 |
| (2,151) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HA | 14 | 0.46 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 7 | 0.46 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 8 | 0.46 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 1 | 0.46 |
| (1,30) | 1:35:A:LEU:HD22 | 1:36:A:LEU:H | 3 | 0.46 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 8 | 0.46 |
| (2,1290) | 1:60:A:ILE:HD11 | 1:19:A:CYS:H | 19 | 0.45 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 19 | 0.45 |
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 10 | 0.45 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 11 | 0.45 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 6 | 0.45 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 19 | 0.45 |
| (2,997) | 1:60:A:ILE:HD13 | 1:69:A:THR:H | 8 | 0.45 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 5 | 0.45 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 8 | 0.45 |
| (2,865) | 1:74:A:VAL:H | 1:15:A:LYS:HE3 | 11 | 0.45 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 3 | 0.45 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 5 | 0.45 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG21 | 18 | 0.45 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 16 | 0.45 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 19 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 5 | 0.45 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 11 | 0.45 |
| (2,504) | 1:7:A:LYS:HD3 | 1:7:A:LYS:HA | 16 | 0.45 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 12 | 0.45 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 17 | 0.45 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 18 | 0.45 |
| (2,337) | 1:52:A:ILE:H | 1:51:A:GLN:HG3 | 2 | 0.45 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG23 | 11 | 0.45 |
| (2,247) | 1:59:A:ALA:HB1 | 1:58:A:ILE:HG21 | 14 | 0.45 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG21 | 5 | 0.45 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 11 | 0.45 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG23 | 18 | 0.45 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 20 | 0.45 |
| (2,124) | 1:86:A:PRO:HG3 | 1:86:A:PRO:HA | 3 | 0.45 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 10 | 0.45 |
| (2,1290) | 1:60:A:ILE:HD13 | 1:19:A:CYS:H | 9 | 0.44 |
| (2,1290) | 1:60:A:ILE:HD11 | 1:19:A:CYS:H | 20 | 0.44 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 15 | 0.44 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 4 | 0.44 |
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 15 | 0.44 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 4 | 0.44 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 13 | 0.44 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 20 | 0.44 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 1 | 0.44 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 16 | 0.44 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 6 | 0.44 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 15 | 0.44 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG23 | 19 | 0.44 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 2 | 0.44 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 18 | 0.44 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 1 | 0.44 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 2 | 0.44 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 4 | 0.44 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 10 | 0.44 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 14 | 0.44 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 3 | 0.44 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 4 | 0.44 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 6 | 0.44 |
| (2,600) | 1:47:A:ILE:HD11 | 1:21:A:THR:HB | 18 | 0.44 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 4 | 0.44 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 5 | 0.44 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 9 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 11 | 0.44 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 18 | 0.44 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 13 | 0.44 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 17 | 0.44 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 20 | 0.44 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 2 | 0.44 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 10 | 0.44 |
| (2,1290) | 1:60:A:ILE:HD13 | 1:19:A:CYS:H | 8 | 0.43 |
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 6 | 0.43 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 8 | 0.43 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 9 | 0.43 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 16 | 0.43 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 16 | 0.43 |
| (2,1153) | 1:32:A:GLU:H | 1:32:A:GLU:HG3 | 20 | 0.43 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 12 | 0.43 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 2 | 0.43 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 19 | 0.43 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 6 | 0.43 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 17 | 0.43 |
| (2,966) | 1:43:A:ASP:HB3 | 1:42:A:LEU:H | 2 | 0.43 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 7 | 0.43 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 7 | 0.43 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG22 | 1 | 0.43 |
| (2,843) | 1:41:A:VAL:HG21 | 1:38:A:THR:HA | 1 | 0.43 |
| (2,828) | 1:60:A:ILE:HD12 | 1:64:A:CYS:HB3 | 4 | 0.43 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 15 | 0.43 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 18 | 0.43 |
| (2,790) | 1:60:A:ILE:HD11 | 1:68:A:PRO:HA | 20 | 0.43 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 13 | 0.43 |
| (2,711) | 1:25:A:VAL:HG22 | 1:48:A:GLN:HG2 | 6 | 0.43 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 6 | 0.43 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 2 | 0.43 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 16 | 0.43 |
| (2,502) | 1:58:A:ILE:HG23 | 1:63:A:GLU:HG3 | 13 | 0.43 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 16 | 0.43 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 7 | 0.43 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 2 | 0.43 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 8 | 0.43 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 15 | 0.43 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 4 | 0.43 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 13 | 0.43 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 8 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 10 | 0.43 |
| (2,29) | 1:69:A:THR:HG21 | 1:84:A:CYS:HB2 | 1 | 0.43 |
| (2,29) | 1:69:A:THR:HG23 | 1:84:A:CYS:HB2 | 13 | 0.43 |
| (2,1210) | 1:46:A:ALA:HB3 | 1:26:A:GLN:H | 9 | 0.42 |
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 10 | 0.42 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 14 | 0.42 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 13 | 0.42 |
| (2,1151) | 1:80:A:VAL:HG23 | 1:81:A:GLY:H | 4 | 0.42 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 13 | 0.42 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 20 | 0.42 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 7 | 0.42 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 9 | 0.42 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 15 | 0.42 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 14 | 0.42 |
| (2,1096) | 1:65:A:LYS:HD3 | 1:66:A:ASN:H | 9 | 0.42 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 12 | 0.42 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 9 | 0.42 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 11 | 0.42 |
| (2,997) | 1:60:A:ILE:HD13 | 1:69:A:THR:H | 13 | 0.42 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 5 | 0.42 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 17 | 0.42 |
| (2,843) | 1:41:A:VAL:HG21 | 1:38:A:THR:HA | 10 | 0.42 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 12 | 0.42 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 14 | 0.42 |
| (2,815) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB3 | 17 | 0.42 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG22 | 8 | 0.42 |
| (2,711) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HG2 | 11 | 0.42 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 13 | 0.42 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 1 | 0.42 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 8 | 0.42 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 15 | 0.42 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 18 | 0.42 |
| (2,611) | 1:85:A:THR:HG21 | 1:86:A:PRO:HD3 | 19 | 0.42 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 7 | 0.42 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG22 | 2 | 0.42 |
| (2,457) | 1:28:A:SER:HB2 | 1:28:A:SER:HA | 6 | 0.42 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 11 | 0.42 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 3 | 0.42 |
| (2,298) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HB3 | 13 | 0.42 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG21 | 3 | 0.42 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG21 | 18 | 0.42 |
| (2,204) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HG2 | 20 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,180) | 1:69:A:THR:HG21 | 1:86:A:PRO:HB2 | 15 | 0.42 |
| (2,180) | 1:69:A:THR:HG22 | 1:86:A:PRO:HB2 | 16 | 0.42 |
| (2,180) | 1:69:A:THR:HG21 | 1:86:A:PRO:HB2 | 18 | 0.42 |
| (2,175) | 1:82:A:ILE:H | 1:82:A:ILE:HG22 | 19 | 0.42 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 18 | 0.42 |
| (1,30) | 1:35:A:LEU:HD22 | 1:36:A:LEU:H | 17 | 0.42 |
| (1,30) | 1:35:A:LEU:HD11 | 1:36:A:LEU:H | 18 | 0.42 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 17 | 0.42 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 1 | 0.41 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 12 | 0.41 |
| (2,1151) | 1:80:A:VAL:HG23 | 1:81:A:GLY:H | 2 | 0.41 |
| (2,1151) | 1:80:A:VAL:HG23 | 1:81:A:GLY:H | 7 | 0.41 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 5 | 0.41 |
| (2,1124) | 1:41:A:VAL:HG21 | 1:44:A:GLN:HE22 | 17 | 0.41 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 17 | 0.41 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 2 | 0.41 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD12 | 9 | 0.41 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 3 | 0.41 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 4 | 0.41 |
| (2,879) | 1:59:A:ALA:H | 1:62:A:ASP:HB3 | 10 | 0.41 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD11 | 13 | 0.41 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 9 | 0.41 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD12 | 16 | 0.41 |
| (2,754) | 1:5:A:GLU:H | 1:5:A:GLU:HG2 | 11 | 0.41 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 7 | 0.41 |
| (2,661) | 1:74:A:VAL:HG13 | 1:78:A:GLY:HA3 | 18 | 0.41 |
| (2,651) | 1:65:A:LYS:HG3 | 1:65:A:LYS:HA | 11 | 0.41 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 7 | 0.41 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 17 | 0.41 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 16 | 0.41 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG23 | 20 | 0.41 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 1 | 0.41 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG22 | 6 | 0.41 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 20 | 0.41 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 2 | 0.41 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 11 | 0.41 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 12 | 0.41 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 1 | 0.41 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 3 | 0.41 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 7 | 0.41 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 13 | 0.41 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 14 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 17 | 0.41 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 20 | 0.41 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 4 | 0.41 |
| (2,151) | 1:60:A:ILE:HD11 | 1:60:A:ILE:HA | 4 | 0.41 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 10 | 0.41 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 11 | 0.41 |
| (2,29) | 1:69:A:THR:HG21 | 1:84:A:CYS:HB2 | 12 | 0.41 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 10 | 0.4 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 19 | 0.4 |
| (2,1210) | 1:46:A:ALA:HB2 | 1:26:A:GLN:H | 13 | 0.4 |
| (2,1196) | 1:35:A:LEU:H | 1:34:A:GLY:HA3 | 1 | 0.4 |
| (2,1196) | 1:35:A:LEU:H | 1:34:A:GLY:HA3 | 15 | 0.4 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 5 | 0.4 |
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 11 | 0.4 |
| (2,1106) | 1:4:A:TRP:H | 1:4:A:TRP:HB3 | 17 | 0.4 |
| (2,1032) | 1:87:A:ILE:HG22 | 1:10:A:SER:H | 16 | 0.4 |
| (2,1016) | 1:82:A:ILE:HG22 | 1:44:A:GLN:H | 6 | 0.4 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 20 | 0.4 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 4 | 0.4 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 14 | 0.4 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG21 | 18 | 0.4 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 2 | 0.4 |
| (2,907) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HG3 | 16 | 0.4 |
| (2,907) | 1:60:A:ILE:HG21 | 1:61:A:GLU:HG3 | 19 | 0.4 |
| (2,906) | 1:7:A:LYS:HG3 | 1:8:A:THR:HA | 20 | 0.4 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 5 | 0.4 |
| (2,843) | 1:41:A:VAL:HG21 | 1:38:A:THR:HA | 20 | 0.4 |
| (2,828) | 1:60:A:ILE:HD13 | 1:64:A:CYS:HB3 | 6 | 0.4 |
| (2,828) | 1:60:A:ILE:HD12 | 1:64:A:CYS:HB3 | 17 | 0.4 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 19 | 0.4 |
| (2,745) | 1:49:A:CYS:H | 1:48:A:GLN:HG3 | 14 | 0.4 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 8 | 0.4 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 10 | 0.4 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 9 | 0.4 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 13 | 0.4 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 5 | 0.4 |
| (2,425) | 1:72:A:GLU:HA | 1:72:A:GLU:HG3 | 10 | 0.4 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 5 | 0.4 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 11 | 0.4 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 6 | 0.4 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 5 | 0.4 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 9 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 19 | 0.39 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 9 | 0.39 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 20 | 0.39 |
| (2,1090) | 1:80:A:VAL:HG12 | 1:48:A:GLN:HE22 | 6 | 0.39 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 5 | 0.39 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 8 | 0.39 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 19 | 0.39 |
| (2,966) | 1:43:A:ASP:HB3 | 1:42:A:LEU:H | 14 | 0.39 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 3 | 0.39 |
| (2,790) | 1:60:A:ILE:HD13 | 1:68:A:PRO:HA | 9 | 0.39 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD13 | 10 | 0.39 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD11 | 19 | 0.39 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 15 | 0.39 |
| (2,759) | 1:75:A:GLU:HA | 1:75:A:GLU:HG2 | 5 | 0.39 |
| (2,754) | 1:5:A:GLU:H | 1:5:A:GLU:HG2 | 2 | 0.39 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 16 | 0.39 |
| (2,502) | 1:58:A:ILE:HG22 | 1:63:A:GLU:HG3 | 2 | 0.39 |
| (2,416) | 1:67:A:THR:HG21 | 1:86:A:PRO:HG3 | 4 | 0.39 |
| (2,393) | 1:19:A:CYS:HB2 | 1:49:A:CYS:HA | 17 | 0.39 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 8 | 0.39 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 9 | 0.39 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG21 | 14 | 0.39 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 8 | 0.39 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 1 | 0.39 |
| (2,1210) | 1:46:A:ALA:HB1 | 1:26:A:GLN:H | 5 | 0.38 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 3 | 0.38 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 14 | 0.38 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 16 | 0.38 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 6 | 0.38 |
| (2,932) | 1:43:A:ASP:HB3 | 1:43:A:ASP:H | 14 | 0.38 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD11 | 19 | 0.38 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 1 | 0.38 |
| (2,828) | 1:60:A:ILE:HD13 | 1:64:A:CYS:HB3 | 10 | 0.38 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 7 | 0.38 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 8 | 0.38 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 11 | 0.38 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 18 | 0.38 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 4 | 0.38 |
| (2,541) | 1:87:A:ILE:HG22 | 1:10:A:SER:HA | 5 | 0.38 |
| (2,541) | 1:87:A:ILE:HG21 | 1:10:A:SER:HA | 6 | 0.38 |
| (2,541) | 1:87:A:ILE:HG23 | 1:10:A:SER:HA | 10 | 0.38 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 8 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 14 | 0.38 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 2 | 0.38 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 10 | 0.38 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 12 | 0.38 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 13 | 0.38 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 2 | 0.38 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 11 | 0.38 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 3 | 0.38 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG21 | 5 | 0.38 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 11 | 0.38 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 3 | 0.38 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 20 | 0.38 |
| (1,30) | 1:35:A:LEU:HD12 | 1:36:A:LEU:H | 19 | 0.38 |
| (1,16) | 1:7:A:LYS:HE3 | 1:7:A:LYS:HG3 | 14 | 0.38 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 20 | 0.37 |
| (2,1253) | 1:16:A:LEU:HD11 | 1:4:A:TRP:HE1 | 10 | 0.37 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 15 | 0.37 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 17 | 0.37 |
| (2,1181) | 1:79:A:LEU:HD22 | 1:51:A:GLN:H | 1 | 0.37 |
| (2,1151) | 1:80:A:VAL:HG23 | 1:81:A:GLY:H | 16 | 0.37 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 18 | 0.37 |
| (2,1151) | 1:80:A:VAL:HG23 | 1:81:A:GLY:H | 20 | 0.37 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 2 | 0.37 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 18 | 0.37 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 19 | 0.37 |
| (2,1122) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE22 | 1 | 0.37 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 3 | 0.37 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD11 | 6 | 0.37 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 11 | 0.37 |
| (2,863) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB2 | 1 | 0.37 |
| (2,847) | 1:19:A:CYS:HB3 | 1:21:A:THR:HG21 | 15 | 0.37 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 4 | 0.37 |
| (2,788) | 1:83:A:ASN:H | 1:82:A:ILE:HD12 | 18 | 0.37 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 12 | 0.37 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 6 | 0.37 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 9 | 0.37 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 12 | 0.37 |
| (2,533) | 1:48:A:GLN:HG3 | 1:48:A:GLN:HA | 20 | 0.37 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 7 | 0.37 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 16 | 0.37 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 15 | 0.37 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 17 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,404) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HG2 | 12 | 0.37 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 3 | 0.37 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 4 | 0.37 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 12 | 0.37 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 19 | 0.37 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG21 | 7 | 0.37 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 16 | 0.37 |
| (2,205) | 1:74:A:VAL:HG23 | 1:15:A:LYS:HE3 | 8 | 0.37 |
| (2,109) | 1:13:A:THR:HG23 | 1:12:A:ASN:HB2 | 6 | 0.37 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 8 | 0.37 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 7 | 0.37 |
| (2,1122) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE22 | 13 | 0.36 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD13 | 4 | 0.36 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 2 | 0.36 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 17 | 0.36 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 2 | 0.36 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 17 | 0.36 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 20 | 0.36 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 13 | 0.36 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 3 | 0.36 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 17 | 0.36 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 18 | 0.36 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 13 | 0.36 |
| (2,611) | 1:85:A:THR:HG23 | 1:86:A:PRO:HD3 | 14 | 0.36 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 10 | 0.36 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG22 | 17 | 0.36 |
| (2,474) | 1:60:A:ILE:HA | 1:60:A:ILE:HG23 | 14 | 0.36 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 12 | 0.36 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 5 | 0.36 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 20 | 0.36 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 10 | 0.36 |
| (2,298) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HB3 | 18 | 0.36 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 10 | 0.36 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 5 | 0.36 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 14 | 0.36 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 6 | 0.36 |
| (2,1290) | 1:60:A:ILE:HD12 | 1:19:A:CYS:H | 16 | 0.35 |
| (2,1216) | 1:46:A:ALA:HB3 | 1:83:A:ASN:H | 13 | 0.35 |
| (2,1216) | 1:46:A:ALA:HB3 | 1:83:A:ASN:H | 20 | 0.35 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 4 | 0.35 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 10 | 0.35 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 6 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1143) | 1:25:A:VAL:HG22 | 1:24:A:LYS:H | 17 | 0.35 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 6 | 0.35 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 14 | 0.35 |
| (2,1016) | 1:82:A:ILE:HG21 | 1:44:A:GLN:H | 19 | 0.35 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 4 | 0.35 |
| (2,997) | 1:60:A:ILE:HD11 | 1:69:A:THR:H | 19 | 0.35 |
| (2,934) | 1:52:A:ILE:H | 1:52:A:ILE:HG22 | 2 | 0.35 |
| (2,932) | 1:43:A:ASP:HB3 | 1:43:A:ASP:H | 2 | 0.35 |
| (2,932) | 1:43:A:ASP:HB3 | 1:43:A:ASP:H | 18 | 0.35 |
| (2,863) | 1:41:A:VAL:HG13 | 1:40:A:ASP:HB2 | 14 | 0.35 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 10 | 0.35 |
| (2,790) | 1:60:A:ILE:HD13 | 1:68:A:PRO:HA | 8 | 0.35 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 6 | 0.35 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 8 | 0.35 |
| (2,711) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HG2 | 17 | 0.35 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 4 | 0.35 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 5 | 0.35 |
| (2,600) | 1:47:A:ILE:HD11 | 1:21:A:THR:HB | 11 | 0.35 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 9 | 0.35 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 4 | 0.35 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 12 | 0.35 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB3 | 14 | 0.35 |
| (2,448) | 1:43:A:ASP:HA | 1:43:A:ASP:HB2 | 14 | 0.35 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 2 | 0.35 |
| (2,416) | 1:67:A:THR:HG23 | 1:86:A:PRO:HG3 | 15 | 0.35 |
| (2,323) | 1:69:A:THR:HG22 | 1:86:A:PRO:HD2 | 19 | 0.35 |
| (2,254) | 1:82:A:ILE:HG22 | 1:73:A:ASP:HB3 | 16 | 0.35 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG21 | 7 | 0.35 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 9 | 0.35 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 18 | 0.35 |
| (2,77) | 1:88:A:PRO:HD2 | 1:88:A:PRO:HB2 | 12 | 0.35 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD12 | 15 | 0.35 |
| (2,1290) | 1:60:A:ILE:HD12 | 1:19:A:CYS:H | 11 | 0.34 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 2 | 0.34 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 1 | 0.34 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 8 | 0.34 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 5 | 0.34 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 1 | 0.34 |
| (2,1068) | 1:47:A:ILE:HG22 | 1:21:A:THR:H | 1 | 0.34 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 14 | 0.34 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 19 | 0.34 |
| (2,939) | 1:79:A:LEU:HB2 | 1:49:A:CYS:H | 5 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 9 | 0.34 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD13 | 10 | 0.34 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD11 | 18 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 1 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD12 | 4 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 5 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 6 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 8 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 9 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 15 | 0.34 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 16 | 0.34 |
| (2,828) | 1:60:A:ILE:HD12 | 1:64:A:CYS:HB3 | 14 | 0.34 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD11 | 12 | 0.34 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 13 | 0.34 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 6 | 0.34 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 14 | 0.34 |
| (2,611) | 1:85:A:THR:HG22 | 1:86:A:PRO:HD3 | 5 | 0.34 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 9 | 0.34 |
| (2,541) | 1:87:A:ILE:HG23 | 1:10:A:SER:HA | 20 | 0.34 |
| (2,448) | 1:43:A:ASP:HA | 1:43:A:ASP:HB2 | 2 | 0.34 |
| (2,439) | 1:60:A:ILE:HG23 | 1:61:A:GLU:HB3 | 7 | 0.34 |
| (2,439) | 1:60:A:ILE:HG23 | 1:61:A:GLU:HB3 | 12 | 0.34 |
| (2,416) | 1:67:A:THR:HG22 | 1:86:A:PRO:HG3 | 9 | 0.34 |
| (2,416) | 1:67:A:THR:HG22 | 1:86:A:PRO:HG3 | 13 | 0.34 |
| (2,404) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HG2 | 1 | 0.34 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 13 | 0.34 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 3 | 0.34 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 11 | 0.34 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 17 | 0.34 |
| (2,266) | 1:36:A:LEU:HB3 | 1:36:A:LEU:HA | 9 | 0.34 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG23 | 1 | 0.34 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG23 | 4 | 0.34 |
| (2,157) | 1:15:A:LYS:H | 1:15:A:LYS:HG2 | 17 | 0.34 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 20 | 0.34 |
| (1,24) | 1:41:A:VAL:HG12 | 1:42:A:LEU:H | 20 | 0.34 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 2 | 0.34 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 12 | 0.34 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 13 | 0.34 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 16 | 0.34 |
| (2,1163) | 1:50:A:THR:HG22 | 1:20:A:ASP:H | 14 | 0.33 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 11 | 0.33 |
| (2,1124) | 1:41:A:VAL:HG22 | 1:44:A:GLN:HE22 | 14 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 9 | 0.33 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 5 | 0.33 |
| (2,1078) | 1:29:A:THR:HG23 | 1:29:A:THR:H | 3 | 0.33 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 9 | 0.33 |
| (2,1032) | 1:87:A:ILE:HG23 | 1:10:A:SER:H | 13 | 0.33 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 18 | 0.33 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 10 | 0.33 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 19 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 2 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 3 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 7 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD12 | 10 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD13 | 11 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 14 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD12 | 17 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD12 | 18 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 19 | 0.33 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 20 | 0.33 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 20 | 0.33 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 1 | 0.33 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 4 | 0.33 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG22 | 6 | 0.33 |
| (2,711) | 1:25:A:VAL:HG21 | 1:48:A:GLN:HG2 | 3 | 0.33 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 1 | 0.33 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 2 | 0.33 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 8 | 0.33 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB2 | 15 | 0.33 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 1 | 0.33 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 9 | 0.33 |
| (2,600) | 1:47:A:ILE:HD13 | 1:21:A:THR:HB | 19 | 0.33 |
| (2,577) | 1:16:A:LEU:HD11 | 1:11:A:CYS:HB3 | 6 | 0.33 |
| (2,541) | 1:87:A:ILE:HG23 | 1:10:A:SER:HA | 15 | 0.33 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG21 | 5 | 0.33 |
| (2,448) | 1:43:A:ASP:HA | 1:43:A:ASP:HB2 | 18 | 0.33 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 4 | 0.33 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 7 | 0.33 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 15 | 0.33 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 16 | 0.33 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 5 | 0.33 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 7 | 0.33 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 18 | 0.33 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 20 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 14 | 0.33 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 14 | 0.33 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 18 | 0.33 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 6 | 0.33 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 14 | 0.33 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 17 | 0.33 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 3 | 0.33 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 7 | 0.33 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 16 | 0.33 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 12 | 0.33 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 6 | 0.33 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 1 | 0.33 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 7 | 0.33 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 9 | 0.33 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 15 | 0.33 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 18 | 0.33 |
| (2,1292) | 1:67:A:THR:HG22 | 1:21:A:THR:H | 8 | 0.32 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 14 | 0.32 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 4 | 0.32 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 2 | 0.32 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 14 | 0.32 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 9 | 0.32 |
| (2,1032) | 1:87:A:ILE:HG23 | 1:10:A:SER:H | 17 | 0.32 |
| (2,932) | 1:43:A:ASP:HB3 | 1:43:A:ASP:H | 9 | 0.32 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD12 | 13 | 0.32 |
| (2,865) | 1:74:A:VAL:H | 1:15:A:LYS:HE3 | 2 | 0.32 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 12 | 0.32 |
| (2,833) | 1:55:A:LEU:HG | 1:55:A:LEU:HD11 | 13 | 0.32 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD11 | 3 | 0.32 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 6 | 0.32 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 16 | 0.32 |
| (2,790) | 1:60:A:ILE:HD12 | 1:68:A:PRO:HA | 16 | 0.32 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 3 | 0.32 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 5 | 0.32 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 11 | 0.32 |
| (2,713) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB2 | 6 | 0.32 |
| (2,713) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB2 | 7 | 0.32 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 4 | 0.32 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 9 | 0.32 |
| (2,711) | 1:25:A:VAL:HG21 | 1:48:A:GLN:HG2 | 15 | 0.32 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB2 | 5 | 0.32 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB2 | 17 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 8 | 0.32 |
| (2,599) | 1:47:A:ILE:HG22 | 1:21:A:THR:HB | 18 | 0.32 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 20 | 0.32 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 2 | 0.32 |
| (2,536) | 1:80:A:VAL:HG13 | 1:48:A:GLN:HA | 5 | 0.32 |
| (2,431) | 1:62:A:ASP:H | 1:62:A:ASP:HB3 | 5 | 0.32 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 1 | 0.32 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 6 | 0.32 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 10 | 0.32 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 17 | 0.32 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 3 | 0.32 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG22 | 10 | 0.32 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 17 | 0.32 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 5 | 0.32 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 2 | 0.32 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 9 | 0.32 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 20 | 0.32 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 12 | 0.32 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 15 | 0.32 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 10 | 0.32 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD12 | 5 | 0.32 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD12 | 10 | 0.32 |
| (1,14) | 1:42:A:LEU:HA | 1:42:A:LEU:HB2 | 17 | 0.32 |
| (1,7) | 1:41:A:VAL:HG13 | 1:40:A:ASP:HB3 | 13 | 0.32 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 4 | 0.31 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 20 | 0.31 |
| (2,1163) | 1:50:A:THR:HG21 | 1:20:A:ASP:H | 4 | 0.31 |
| (2,1163) | 1:50:A:THR:HG23 | 1:20:A:ASP:H | 12 | 0.31 |
| (2,1143) | 1:25:A:VAL:HG23 | 1:24:A:LYS:H | 13 | 0.31 |
| (2,1078) | 1:29:A:THR:HG21 | 1:29:A:THR:H | 12 | 0.31 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 17 | 0.31 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 7 | 0.31 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 8 | 0.31 |
| (2,973) | 1:47:A:ILE:HG22 | 1:23:A:LYS:H | 3 | 0.31 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD13 | 9 | 0.31 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 1 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 2 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 3 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 4 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 5 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 6 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 8 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 9 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 10 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 11 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 13 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 14 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 15 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 17 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 18 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 19 | 0.31 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 20 | 0.31 |
| (2,863) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB2 | 18 | 0.31 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD13 | 13 | 0.31 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 16 | 0.31 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 9 | 0.31 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD12 | 10 | 0.31 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 14 | 0.31 |
| (2,711) | 1:25:A:VAL:HG22 | 1:48:A:GLN:HG2 | 7 | 0.31 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 11 | 0.31 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 16 | 0.31 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 6 | 0.31 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 9 | 0.31 |
| (2,568) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HB2 | 11 | 0.31 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG22 | 7 | 0.31 |
| (2,459) | 1:45:A:VAL:HG13 | 1:44:A:GLN:HA | 20 | 0.31 |
| (2,448) | 1:43:A:ASP:HA | 1:43:A:ASP:HB2 | 9 | 0.31 |
| (2,439) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HB3 | 6 | 0.31 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 10 | 0.31 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 18 | 0.31 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 6 | 0.31 |
| (2,369) | 1:67:A:THR:HG23 | 1:68:A:PRO:HD3 | 20 | 0.31 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 12 | 0.31 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 14 | 0.31 |
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 7 | 0.31 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 6 | 0.31 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 7 | 0.31 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG22 | 11 | 0.31 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 4 | 0.31 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 9 | 0.31 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 3 | 0.31 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 4 | 0.31 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 10 | 0.31 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 11 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 14 | 0.31 |
| (2,53) | 1:65:A:LYS:HB3 | 1:65:A:LYS:HD3 | 13 | 0.31 |
| (2,1292) | 1:67:A:THR:HG22 | 1:21:A:THR:H | 16 | 0.3 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 6 | 0.3 |
| (2,1131) | 1:23:A:LYS:HG3 | 1:22:A:ASN:H | 15 | 0.3 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 1 | 0.3 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 16 | 0.3 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 13 | 0.3 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 1 | 0.3 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 7 | 0.3 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 12 | 0.3 |
| (2,882) | 1:89:A:LEU:HA | 1:89:A:LEU:HB2 | 16 | 0.3 |
| (2,879) | 1:59:A:ALA:H | 1:62:A:ASP:HB3 | 16 | 0.3 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 4 | 0.3 |
| (2,856) | 1:90:A:ILE:HD11 | 1:88:A:PRO:HG3 | 20 | 0.3 |
| (2,787) | 1:74:A:VAL:H | 1:82:A:ILE:HD12 | 10 | 0.3 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 16 | 0.3 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 4 | 0.3 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 16 | 0.3 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB2 | 20 | 0.3 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 8 | 0.3 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 17 | 0.3 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 18 | 0.3 |
| (2,484) | 1:87:A:ILE:HG23 | 1:88:A:PRO:HD2 | 19 | 0.3 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG21 | 14 | 0.3 |
| (2,459) | 1:45:A:VAL:HG12 | 1:44:A:GLN:HA | 11 | 0.3 |
| (2,379) | 1:82:A:ILE:HG21 | 1:83:A:ASN:HB3 | 1 | 0.3 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 9 | 0.3 |
| (2,369) | 1:67:A:THR:HG23 | 1:68:A:PRO:HD3 | 8 | 0.3 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 19 | 0.3 |
| (2,323) | 1:69:A:THR:HG22 | 1:86:A:PRO:HD2 | 13 | 0.3 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 8 | 0.3 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 9 | 0.3 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 16 | 0.3 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG23 | 18 | 0.3 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 16 | 0.3 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 8 | 0.3 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 11 | 0.3 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 16 | 0.3 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 17 | 0.3 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 19 | 0.3 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 5 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 3 | 0.3 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 15 | 0.3 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 14 | 0.3 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 2 | 0.3 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD13 | 6 | 0.3 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD11 | 11 | 0.3 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD12 | 18 | 0.3 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD23 | 8 | 0.3 |
| (2,1290) | 1:60:A:ILE:HD12 | 1:19:A:CYS:H | 17 | 0.29 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 10 | 0.29 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 8 | 0.29 |
| (2,1151) | 1:80:A:VAL:HG22 | 1:81:A:GLY:H | 5 | 0.29 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 10 | 0.29 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 20 | 0.29 |
| (2,1078) | 1:29:A:THR:HG22 | 1:29:A:THR:H | 2 | 0.29 |
| (2,1078) | 1:29:A:THR:HG22 | 1:29:A:THR:H | 15 | 0.29 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 18 | 0.29 |
| (2,997) | 1:60:A:ILE:HD12 | 1:69:A:THR:H | 11 | 0.29 |
| (2,940) | 1:79:A:LEU:HD23 | 1:49:A:CYS:H | 2 | 0.29 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 3 | 0.29 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD11 | 13 | 0.29 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 2 | 0.29 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 3 | 0.29 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 9 | 0.29 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 14 | 0.29 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD13 | 5 | 0.29 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 13 | 0.29 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 18 | 0.29 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 1 | 0.29 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 9 | 0.29 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD11 | 7 | 0.29 |
| (2,759) | 1:75:A:GLU:HA | 1:75:A:GLU:HG2 | 6 | 0.29 |
| (2,711) | 1:25:A:VAL:HG22 | 1:48:A:GLN:HG2 | 18 | 0.29 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 15 | 0.29 |
| (2,630) | 1:52:A:ILE:HD11 | 1:64:A:CYS:HB3 | 5 | 0.29 |
| (2,624) | 1:74:A:VAL:HG11 | 1:78:A:GLY:HA2 | 8 | 0.29 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 20 | 0.29 |
| (2,603) | 1:16:A:LEU:HD13 | 1:70:A:CYS:HA | 6 | 0.29 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 8 | 0.29 |
| (2,577) | 1:16:A:LEU:HD12 | 1:11:A:CYS:HB3 | 10 | 0.29 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 16 | 0.29 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD22 | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,537) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HA | 20 | 0.29 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 7 | 0.29 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG23 | 11 | 0.29 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB2 | 5 | 0.29 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 7 | 0.29 |
| (2,416) | 1:67:A:THR:HG21 | 1:86:A:PRO:HG3 | 5 | 0.29 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 17 | 0.29 |
| (2,369) | 1:67:A:THR:HG21 | 1:68:A:PRO:HD3 | 14 | 0.29 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 4 | 0.29 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 10 | 0.29 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 15 | 0.29 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 11 | 0.29 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG22 | 12 | 0.29 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 15 | 0.29 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 18 | 0.29 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 19 | 0.29 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 20 | 0.29 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 2 | 0.29 |
| (2,179) | 1:86:A:PRO:HB2 | 1:67:A:THR:HG23 | 14 | 0.29 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 17 | 0.29 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 9 | 0.29 |
| (2,137) | 1:23:A:LYS:HE3 | 1:23:A:LYS:HD3 | 15 | 0.29 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 8 | 0.29 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 16 | 0.29 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG21 | 18 | 0.29 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 1 | 0.29 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 8 | 0.29 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 13 | 0.29 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 2 | 0.29 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 10 | 0.29 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD23 | 14 | 0.29 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 3 | 0.28 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 9 | 0.28 |
| (2,1143) | 1:25:A:VAL:HG21 | 1:24:A:LYS:H | 3 | 0.28 |
| (2,1122) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE22 | 20 | 0.28 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 3 | 0.28 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 6 | 0.28 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 7 | 0.28 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 16 | 0.28 |
| (2,1078) | 1:29:A:THR:HG22 | 1:29:A:THR:H | 17 | 0.28 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 15 | 0.28 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 7 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 17 | 0.28 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD13 | 7 | 0.28 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 4 | 0.28 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 13 | 0.28 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 3 | 0.28 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 8 | 0.28 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 15 | 0.28 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 5 | 0.28 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 8 | 0.28 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 19 | 0.28 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 14 | 0.28 |
| (2,879) | 1:59:A:ALA:H | 1:62:A:ASP:HB3 | 2 | 0.28 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 9 | 0.28 |
| (2,814) | 1:24:A:LYS:H | 1:23:A:LYS:HB3 | 14 | 0.28 |
| (2,776) | 1:44:A:GLN:HE21 | 1:82:A:ILE:HG22 | 12 | 0.28 |
| (2,711) | 1:25:A:VAL:HG21 | 1:48:A:GLN:HG2 | 4 | 0.28 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 18 | 0.28 |
| (2,603) | 1:16:A:LEU:HD11 | 1:70:A:CYS:HA | 12 | 0.28 |
| (2,603) | 1:16:A:LEU:HD11 | 1:70:A:CYS:HA | 16 | 0.28 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 10 | 0.28 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 9 | 0.28 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 19 | 0.28 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 10 | 0.28 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 13 | 0.28 |
| (2,439) | 1:60:A:ILE:HG22 | 1:61:A:GLU:HB3 | 2 | 0.28 |
| (2,439) | 1:60:A:ILE:HG21 | 1:61:A:GLU:HB3 | 5 | 0.28 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 2 | 0.28 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 14 | 0.28 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 19 | 0.28 |
| (2,379) | 1:82:A:ILE:HG23 | 1:83:A:ASN:HB3 | 14 | 0.28 |
| (2,369) | 1:67:A:THR:HG23 | 1:68:A:PRO:HD3 | 2 | 0.28 |
| (2,369) | 1:67:A:THR:HG23 | 1:68:A:PRO:HD3 | 12 | 0.28 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 1 | 0.28 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 2 | 0.28 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 5 | 0.28 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 9 | 0.28 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 14 | 0.28 |
| (2,323) | 1:69:A:THR:HG22 | 1:86:A:PRO:HD2 | 16 | 0.28 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG22 | 12 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 1 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 2 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 3 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 4 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 5 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 6 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 7 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 8 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 10 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 11 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 12 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 13 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 14 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 16 | 0.28 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 17 | 0.28 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 15 | 0.28 |
| (2,180) | 1:69:A:THR:HG21 | 1:86:A:PRO:HB2 | 6 | 0.28 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 1 | 0.28 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 2 | 0.28 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 14 | 0.28 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 16 | 0.28 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 17 | 0.28 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 6 | 0.28 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 2 | 0.28 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 19 | 0.28 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 1 | 0.28 |
| (2,99) | 1:58:A:ILE:HG22 | 1:58:A:ILE:HA | 20 | 0.28 |
| (2,57) | 1:86:A:PRO:HG3 | 1:85:A:THR:HA | 3 | 0.28 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 2 | 0.28 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 3 | 0.28 |
| (1,24) | 1:41:A:VAL:HG13 | 1:42:A:LEU:H | 2 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 5 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD21 | 9 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD23 | 11 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 13 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD23 | 16 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD21 | 18 | 0.28 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 19 | 0.28 |
| (2,1290) | 1:60:A:ILE:HD12 | 1:19:A:CYS:H | 4 | 0.27 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 8 | 0.27 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 20 | 0.27 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 4 | 0.27 |
| (2,1068) | 1:47:A:ILE:HG22 | 1:21:A:THR:H | 5 | 0.27 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 19 | 0.27 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 6 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 7 | 0.27 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 9 | 0.27 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 15 | 0.27 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 17 | 0.27 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 18 | 0.27 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 11 | 0.27 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 7 | 0.27 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 16 | 0.27 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 8 | 0.27 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG22 | 15 | 0.27 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 2 | 0.27 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 5 | 0.27 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 16 | 0.27 |
| (2,856) | 1:90:A:ILE:HD11 | 1:88:A:PRO:HG3 | 17 | 0.27 |
| (2,825) | 1:8:A:THR:HG22 | 1:10:A:SER:HB3 | 5 | 0.27 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 3 | 0.27 |
| (2,785) | 1:73:A:ASP:HB2 | 1:82:A:ILE:HD13 | 19 | 0.27 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG21 | 15 | 0.27 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 10 | 0.27 |
| (2,615) | 1:46:A:ALA:HB3 | 1:25:A:VAL:HG22 | 15 | 0.27 |
| (2,599) | 1:47:A:ILE:HG22 | 1:21:A:THR:HB | 4 | 0.27 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 7 | 0.27 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 5 | 0.27 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 10 | 0.27 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 5 | 0.27 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB2 | 17 | 0.27 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG22 | 17 | 0.27 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 8 | 0.27 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 10 | 0.27 |
| (2,489) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HB | 4 | 0.27 |
| (2,476) | 1:4:A:TRP:HB2 | 1:60:A:ILE:HG23 | 17 | 0.27 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 4 | 0.27 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 3 | 0.27 |
| (2,379) | 1:82:A:ILE:HG22 | 1:83:A:ASN:HB3 | 10 | 0.27 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 6 | 0.27 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 1 | 0.27 |
| (2,298) | 1:47:A:ILE:HG21 | 1:24:A:LYS:HB3 | 5 | 0.27 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG23 | 13 | 0.27 |
| (2,219) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HA | 9 | 0.27 |
| (2,180) | 1:69:A:THR:HG22 | 1:86:A:PRO:HB2 | 19 | 0.27 |
| (2,172) | 1:44:A:GLN:HB2 | 1:82:A:ILE:HG23 | 12 | 0.27 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 11 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 14 | 0.27 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 9 | 0.27 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 11 | 0.27 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 18 | 0.27 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 19 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 2 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 3 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 5 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 6 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 7 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 8 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 9 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 10 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 11 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 12 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 13 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 16 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 18 | 0.27 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 20 | 0.27 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD13 | 19 | 0.27 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD23 | 4 | 0.27 |
| (1,3) | 1:35:A:LEU:HG | 1:35:A:LEU:HD22 | 15 | 0.27 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 1 | 0.26 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 7 | 0.26 |
| (2,1181) | 1:79:A:LEU:HD22 | 1:51:A:GLN:H | 4 | 0.26 |
| (2,1163) | 1:50:A:THR:HG23 | 1:20:A:ASP:H | 19 | 0.26 |
| (2,1141) | 1:24:A:LYS:H | 1:24:A:LYS:HG2 | 15 | 0.26 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 18 | 0.26 |
| (2,1078) | 1:29:A:THR:HG22 | 1:29:A:THR:H | 8 | 0.26 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 9 | 0.26 |
| (2,997) | 1:60:A:ILE:HD12 | 1:69:A:THR:H | 1 | 0.26 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD13 | 3 | 0.26 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 5 | 0.26 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 11 | 0.26 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 16 | 0.26 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 4 | 0.26 |
| (2,911) | 1:61:A:GLU:HA | 1:61:A:GLU:HG2 | 9 | 0.26 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 16 | 0.26 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 12 | 0.26 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 13 | 0.26 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 15 | 0.26 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 20 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 1 | 0.26 |
| (2,856) | 1:90:A:ILE:HD11 | 1:88:A:PRO:HG3 | 3 | 0.26 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 7 | 0.26 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 14 | 0.26 |
| (2,822) | 1:87:A:ILE:H | 1:87:A:ILE:HD12 | 5 | 0.26 |
| (2,814) | 1:24:A:LYS:H | 1:23:A:LYS:HB3 | 20 | 0.26 |
| (2,790) | 1:60:A:ILE:HD11 | 1:68:A:PRO:HA | 19 | 0.26 |
| (2,711) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HG2 | 10 | 0.26 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 7 | 0.26 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 9 | 0.26 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 13 | 0.26 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 4 | 0.26 |
| (2,603) | 1:16:A:LEU:HD11 | 1:70:A:CYS:HA | 18 | 0.26 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 11 | 0.26 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 12 | 0.26 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 19 | 0.26 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 17 | 0.26 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 13 | 0.26 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD22 | 14 | 0.26 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 10 | 0.26 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG23 | 17 | 0.26 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 12 | 0.26 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 12 | 0.26 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 9 | 0.26 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD11 | 17 | 0.26 |
| (2,369) | 1:67:A:THR:HG22 | 1:68:A:PRO:HD3 | 10 | 0.26 |
| (2,336) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HG3 | 15 | 0.26 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 13 | 0.26 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 16 | 0.26 |
| (2,323) | 1:69:A:THR:HG23 | 1:86:A:PRO:HD2 | 5 | 0.26 |
| (2,323) | 1:69:A:THR:HG22 | 1:86:A:PRO:HD2 | 9 | 0.26 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 16 | 0.26 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 19 | 0.26 |
| (2,239) | 1:87:A:ILE:HG23 | 1:70:A:CYS:HB2 | 4 | 0.26 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG22 | 2 | 0.26 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 12 | 0.26 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 4 | 0.26 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 11 | 0.26 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 11 | 0.26 |
| (2,180) | 1:69:A:THR:HG22 | 1:86:A:PRO:HB2 | 13 | 0.26 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 10 | 0.26 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 13 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 19 | 0.26 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 20 | 0.26 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG22 | 9 | 0.26 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 2 | 0.26 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 4 | 0.26 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 6 | 0.26 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 14 | 0.26 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 16 | 0.26 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 7 | 0.26 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 12 | 0.26 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 1 | 0.26 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 4 | 0.26 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 14 | 0.26 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 19 | 0.26 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD11 | 3 | 0.26 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD11 | 17 | 0.26 |
| (1,14) | 1:42:A:LEU:HG | 1:42:A:LEU:HA | 11 | 0.26 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD22 | 17 | 0.26 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 6 | 0.25 |
| (2,1216) | 1:46:A:ALA:HB3 | 1:83:A:ASN:H | 12 | 0.25 |
| (2,1163) | 1:50:A:THR:HG23 | 1:20:A:ASP:H | 3 | 0.25 |
| (2,1151) | 1:80:A:VAL:HG21 | 1:81:A:GLY:H | 15 | 0.25 |
| (2,1122) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE22 | 11 | 0.25 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 17 | 0.25 |
| (2,1068) | 1:47:A:ILE:HG22 | 1:21:A:THR:H | 18 | 0.25 |
| (2,1016) | 1:82:A:ILE:HG23 | 1:44:A:GLN:H | 16 | 0.25 |
| (2,999) | 1:87:A:ILE:HG13 | 1:69:A:THR:H | 15 | 0.25 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD13 | 2 | 0.25 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 1 | 0.25 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 3 | 0.25 |
| (2,889) | 1:47:A:ILE:HD13 | 1:19:A:CYS:HA | 5 | 0.25 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 6 | 0.25 |
| (2,887) | 1:12:A:ASN:HD22 | 1:12:A:ASN:HA | 18 | 0.25 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 14 | 0.25 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 2 | 0.25 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 3 | 0.25 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG22 | 7 | 0.25 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 11 | 0.25 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 7 | 0.25 |
| (2,858) | 1:51:A:GLN:HE22 | 1:51:A:GLN:HA | 17 | 0.25 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 4 | 0.25 |
| (2,720) | 1:82:A:ILE:HG23 | 1:44:A:GLN:HA | 12 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 12 | 0.25 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 12 | 0.25 |
| (2,666) | 1:84:A:CYS:HB3 | 1:71:A:CYS:HA | 1 | 0.25 |
| (2,666) | 1:84:A:CYS:HB3 | 1:71:A:CYS:HA | 12 | 0.25 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 10 | 0.25 |
| (2,624) | 1:74:A:VAL:HG13 | 1:78:A:GLY:HA2 | 18 | 0.25 |
| (2,600) | 1:47:A:ILE:HD11 | 1:21:A:THR:HB | 12 | 0.25 |
| (2,599) | 1:47:A:ILE:HG22 | 1:21:A:THR:HB | 1 | 0.25 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 2 | 0.25 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 20 | 0.25 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB1 | 3 | 0.25 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 6 | 0.25 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG21 | 12 | 0.25 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 18 | 0.25 |
| (2,471) | 1:61:A:GLU:HG3 | 1:59:A:ALA:HB1 | 6 | 0.25 |
| (2,451) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB2 | 16 | 0.25 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 9 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 1 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 2 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 3 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 6 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 7 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 10 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 13 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 15 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 16 | 0.25 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 20 | 0.25 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 2 | 0.25 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 8 | 0.25 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 13 | 0.25 |
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 13 | 0.25 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 15 | 0.25 |
| (2,260) | 1:69:A:THR:HG22 | 1:19:A:CYS:HB3 | 6 | 0.25 |
| (2,260) | 1:69:A:THR:HG22 | 1:19:A:CYS:HB3 | 18 | 0.25 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG23 | 5 | 0.25 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG22 | 7 | 0.25 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 17 | 0.25 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 18 | 0.25 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 19 | 0.25 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 20 | 0.25 |
| (2,193) | 1:24:A:LYS:HG3 | 1:24:A:LYS:HA | 4 | 0.25 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 1 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 12 | 0.25 |
| (2,141) | 1:27:A:LYS:HD3 | 1:27:A:LYS:HE3 | 8 | 0.25 |
| (2,124) | 1:86:A:PRO:HG3 | 1:86:A:PRO:HA | 13 | 0.25 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG21 | 4 | 0.25 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG21 | 5 | 0.25 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 7 | 0.25 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 10 | 0.25 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 15 | 0.25 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD12 | 8 | 0.25 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 4 | 0.25 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 10 | 0.25 |
| (1,16) | 1:7:A:LYS:HE2 | 1:7:A:LYS:HG3 | 2 | 0.25 |
| (1,14) | 1:42:A:LEU:HG | 1:42:A:LEU:HA | 3 | 0.25 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD22 | 12 | 0.25 |
| (2,1292) | 1:67:A:THR:HG22 | 1:21:A:THR:H | 9 | 0.24 |
| (2,1292) | 1:67:A:THR:HG22 | 1:21:A:THR:H | 20 | 0.24 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 2 | 0.24 |
| (2,1255) | 1:82:A:ILE:HD12 | 1:44:A:GLN:HE21 | 3 | 0.24 |
| (2,1199) | 1:56:A:ILE:HG12 | 1:57:A:GLY:H | 6 | 0.24 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 15 | 0.24 |
| (2,1163) | 1:50:A:THR:HG21 | 1:20:A:ASP:H | 9 | 0.24 |
| (2,1131) | 1:23:A:LYS:HG3 | 1:22:A:ASN:H | 14 | 0.24 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 9 | 0.24 |
| (2,1078) | 1:29:A:THR:HG21 | 1:29:A:THR:H | 19 | 0.24 |
| (2,1076) | 1:29:A:THR:H | 1:28:A:SER:HA | 6 | 0.24 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 19 | 0.24 |
| (2,1032) | 1:87:A:ILE:HG21 | 1:10:A:SER:H | 3 | 0.24 |
| (2,966) | 1:43:A:ASP:HB3 | 1:42:A:LEU:H | 18 | 0.24 |
| (2,939) | 1:79:A:LEU:HB2 | 1:49:A:CYS:H | 9 | 0.24 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 8 | 0.24 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 6 | 0.24 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 7 | 0.24 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 15 | 0.24 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 15 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 13 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 14 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 16 | 0.24 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 18 | 0.24 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD11 | 15 | 0.24 |
| (2,856) | 1:90:A:ILE:HD12 | 1:88:A:PRO:HG3 | 6 | 0.24 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 2 | 0.24 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 14 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,814) | 1:24:A:LYS:H | 1:23:A:LYS:HB3 | 15 | 0.24 |
| (2,754) | 1:5:A:GLU:H | 1:5:A:GLU:HG2 | 12 | 0.24 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 9 | 0.24 |
| (2,630) | 1:52:A:ILE:HD12 | 1:64:A:CYS:HB3 | 2 | 0.24 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 5 | 0.24 |
| (2,603) | 1:16:A:LEU:HD13 | 1:70:A:CYS:HA | 7 | 0.24 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 3 | 0.24 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 6 | 0.24 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 13 | 0.24 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD21 | 8 | 0.24 |
| (2,520) | 1:56:A:ILE:H | 1:56:A:ILE:HG12 | 8 | 0.24 |
| (2,503) | 1:7:A:LYS:HB3 | 1:7:A:LYS:HA | 17 | 0.24 |
| (2,484) | 1:87:A:ILE:HG23 | 1:88:A:PRO:HD2 | 15 | 0.24 |
| (2,459) | 1:45:A:VAL:HG11 | 1:44:A:GLN:HA | 8 | 0.24 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 4 | 0.24 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 5 | 0.24 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 12 | 0.24 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 14 | 0.24 |
| (2,435) | 1:26:A:GLN:HG2 | 1:26:A:GLN:HB2 | 18 | 0.24 |
| (2,369) | 1:67:A:THR:HG21 | 1:68:A:PRO:HD3 | 19 | 0.24 |
| (2,352) | 1:49:A:CYS:HB2 | 1:19:A:CYS:HA | 9 | 0.24 |
| (2,289) | 1:23:A:LYS:HB3 | 1:20:A:ASP:HB2 | 9 | 0.24 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB2 | 17 | 0.24 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 11 | 0.24 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG21 | 14 | 0.24 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 5 | 0.24 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 10 | 0.24 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 2 | 0.24 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 6 | 0.24 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 10 | 0.24 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 16 | 0.24 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 16 | 0.24 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 5 | 0.24 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 10 | 0.24 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 10 | 0.24 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 4 | 0.24 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 4 | 0.24 |
| (2,124) | 1:86:A:PRO:HG3 | 1:86:A:PRO:HA | 5 | 0.24 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 5 | 0.24 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 7 | 0.24 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 12 | 0.24 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 3 | 0.24 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 7 | 0.24 |
| (1,7) | 1:41:A:VAL:HG11 | 1:40:A:ASP:HB3 | 12 | 0.24 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD22 | 3 | 0.24 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 13 | 0.23 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 2 | 0.23 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 18 | 0.23 |
| (2,1078) | 1:29:A:THR:HG21 | 1:29:A:THR:H | 9 | 0.23 |
| (2,1068) | 1:47:A:ILE:HG21 | 1:21:A:THR:H | 6 | 0.23 |
| (2,940) | 1:79:A:LEU:HD23 | 1:49:A:CYS:H | 13 | 0.23 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD11 | 1 | 0.23 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 11 | 0.23 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 9 | 0.23 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 11 | 0.23 |
| (2,885) | 1:47:A:ILE:HD13 | 1:47:A:ILE:HA | 16 | 0.23 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 1 | 0.23 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG21 | 12 | 0.23 |
| (2,722) | 1:87:A:ILE:HG21 | 1:70:A:CYS:HB3 | 10 | 0.23 |
| (2,713) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB2 | 5 | 0.23 |
| (2,713) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB2 | 17 | 0.23 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 18 | 0.23 |
| (2,666) | 1:84:A:CYS:HB3 | 1:71:A:CYS:HA | 13 | 0.23 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 1 | 0.23 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 12 | 0.23 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 16 | 0.23 |
| (2,650) | 1:65:A:LYS:HA | 1:65:A:LYS:HD3 | 18 | 0.23 |
| (2,630) | 1:52:A:ILE:HD12 | 1:64:A:CYS:HB3 | 10 | 0.23 |
| (2,630) | 1:52:A:ILE:HD12 | 1:64:A:CYS:HB3 | 11 | 0.23 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 10 | 0.23 |
| (2,617) | 1:26:A:GLN:HB3 | 1:27:A:LYS:HG2 | 17 | 0.23 |
| (2,603) | 1:16:A:LEU:HD11 | 1:70:A:CYS:HA | 2 | 0.23 |
| (2,603) | 1:16:A:LEU:HD13 | 1:70:A:CYS:HA | 3 | 0.23 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 9 | 0.23 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 11 | 0.23 |
| (2,603) | 1:16:A:LEU:HD13 | 1:70:A:CYS:HA | 17 | 0.23 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 19 | 0.23 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 16 | 0.23 |
| (2,568) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HB2 | 12 | 0.23 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD13 | 17 | 0.23 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG22 | 3 | 0.23 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG22 | 19 | 0.23 |
| (2,439) | 1:60:A:ILE:HG23 | 1:61:A:GLU:HB3 | 14 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 6 | 0.23 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 18 | 0.23 |
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 17 | 0.23 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 10 | 0.23 |
| (2,260) | 1:69:A:THR:HG23 | 1:19:A:CYS:HB3 | 19 | 0.23 |
| (2,228) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA3 | 19 | 0.23 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 1 | 0.23 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 7 | 0.23 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 8 | 0.23 |
| (2,213) | 1:86:A:PRO:HD2 | 1:85:A:THR:HA | 12 | 0.23 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 4 | 0.23 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 6 | 0.23 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 13 | 0.23 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 15 | 0.23 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 16 | 0.23 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 8 | 0.23 |
| (2,124) | 1:86:A:PRO:HG3 | 1:86:A:PRO:HA | 14 | 0.23 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG21 | 1 | 0.23 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 18 | 0.23 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 15 | 0.23 |
| (2,99) | 1:58:A:ILE:HG21 | 1:58:A:ILE:HA | 17 | 0.23 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 17 | 0.23 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 18 | 0.23 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD22 | 20 | 0.23 |
| (2,1290) | 1:60:A:ILE:HD13 | 1:19:A:CYS:H | 13 | 0.22 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 11 | 0.22 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 11 | 0.22 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 15 | 0.22 |
| (2,1159) | 1:47:A:ILE:HG22 | 1:46:A:ALA:H | 7 | 0.22 |
| (2,1083) | 1:26:A:GLN:HB2 | 1:26:A:GLN:HE21 | 4 | 0.22 |
| (2,1068) | 1:47:A:ILE:HG21 | 1:21:A:THR:H | 7 | 0.22 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 7 | 0.22 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 11 | 0.22 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 13 | 0.22 |
| (2,923) | 1:21:A:THR:HG22 | 1:67:A:THR:HB | 19 | 0.22 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD12 | 15 | 0.22 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD11 | 17 | 0.22 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD12 | 14 | 0.22 |
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 3 | 0.22 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 17 | 0.22 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 7 | 0.22 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,821) | 1:11:A:CYS:H | 1:10:A:SER:HB3 | 6 | 0.22 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 10 | 0.22 |
| (2,720) | 1:82:A:ILE:HG21 | 1:44:A:GLN:HA | 5 | 0.22 |
| (2,720) | 1:82:A:ILE:HG22 | 1:44:A:GLN:HA | 7 | 0.22 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB3 | 4 | 0.22 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 2 | 0.22 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 5 | 0.22 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 7 | 0.22 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 9 | 0.22 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 10 | 0.22 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 8 | 0.22 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 1 | 0.22 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 13 | 0.22 |
| (2,599) | 1:47:A:ILE:HG22 | 1:21:A:THR:HB | 13 | 0.22 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 14 | 0.22 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 2 | 0.22 |
| (2,589) | 1:15:A:LYS:H | 1:14:A:GLY:HA2 | 14 | 0.22 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 16 | 0.22 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD22 | 4 | 0.22 |
| (2,541) | 1:87:A:ILE:HG23 | 1:10:A:SER:HA | 2 | 0.22 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG22 | 15 | 0.22 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 16 | 0.22 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 6 | 0.22 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 1 | 0.22 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 14 | 0.22 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD13 | 3 | 0.22 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 4 | 0.22 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD13 | 7 | 0.22 |
| (2,332) | 1:67:A:THR:H | 1:66:A:ASN:HB2 | 8 | 0.22 |
| (2,317) | 1:23:A:LYS:H | 1:22:A:ASN:HB2 | 20 | 0.22 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB1 | 10 | 0.22 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 17 | 0.22 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG23 | 13 | 0.22 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 16 | 0.22 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 20 | 0.22 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 9 | 0.22 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 17 | 0.22 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 3 | 0.22 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 16 | 0.22 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 17 | 0.22 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 18 | 0.22 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 11 | 0.22 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 3 | 0.22 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 15 | 0.22 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 13 | 0.22 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 3 | 0.22 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 2 | 0.22 |
| (2,79) | 1:63:A:GLU:H | 1:63:A:GLU:HB2 | 12 | 0.22 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 2 | 0.22 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 6 | 0.22 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 9 | 0.22 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 13 | 0.22 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 16 | 0.22 |
| (2,52) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HD3 | 18 | 0.22 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD13 | 13 | 0.22 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD21 | 6 | 0.22 |
| (2,1290) | 1:60:A:ILE:HD13 | 1:19:A:CYS:H | 2 | 0.21 |
| (2,1290) | 1:60:A:ILE:HD11 | 1:19:A:CYS:H | 5 | 0.21 |
| (2,1273) | 1:24:A:LYS:H | 1:24:A:LYS:HD3 | 12 | 0.21 |
| (2,1213) | 1:45:A:VAL:HG23 | 1:83:A:ASN:H | 16 | 0.21 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 19 | 0.21 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 6 | 0.21 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 11 | 0.21 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 12 | 0.21 |
| (2,1162) | 1:88:A:PRO:HG3 | 1:89:A:LEU:H | 12 | 0.21 |
| (2,1153) | 1:32:A:GLU:H | 1:32:A:GLU:HG3 | 8 | 0.21 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 2 | 0.21 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 13 | 0.21 |
| (2,1078) | 1:29:A:THR:HG21 | 1:29:A:THR:H | 20 | 0.21 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 9 | 0.21 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 1 | 0.21 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 4 | 0.21 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 5 | 0.21 |
| (2,885) | 1:47:A:ILE:HD13 | 1:47:A:ILE:HA | 8 | 0.21 |
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 20 | 0.21 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 4 | 0.21 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG22 | 6 | 0.21 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 17 | 0.21 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 20 | 0.21 |
| (2,856) | 1:90:A:ILE:HD11 | 1:88:A:PRO:HG3 | 19 | 0.21 |
| (2,835) | 1:69:A:THR:H | 1:69:A:THR:HG22 | 12 | 0.21 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 11 | 0.21 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 8 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,715) | 1:15:A:LYS:HE3 | 1:15:A:LYS:HB2 | 15 | 0.21 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 2 | 0.21 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 8 | 0.21 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 19 | 0.21 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 20 | 0.21 |
| (2,696) | 1:50:A:THR:H | 1:17:A:ALA:HB1 | 19 | 0.21 |
| (2,661) | 1:74:A:VAL:HG13 | 1:78:A:GLY:HA3 | 15 | 0.21 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 8 | 0.21 |
| (2,652) | 1:65:A:LYS:HA | 1:65:A:LYS:HB3 | 18 | 0.21 |
| (2,603) | 1:16:A:LEU:HD13 | 1:70:A:CYS:HA | 20 | 0.21 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 10 | 0.21 |
| (2,599) | 1:47:A:ILE:HG21 | 1:21:A:THR:HB | 15 | 0.21 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 17 | 0.21 |
| (2,599) | 1:47:A:ILE:HG23 | 1:21:A:THR:HB | 20 | 0.21 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 2 | 0.21 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 4 | 0.21 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 11 | 0.21 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD22 | 6 | 0.21 |
| (2,543) | 1:79:A:LEU:HD22 | 1:50:A:THR:HA | 13 | 0.21 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD13 | 2 | 0.21 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG23 | 9 | 0.21 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG21 | 9 | 0.21 |
| (2,477) | 1:61:A:GLU:HB2 | 1:60:A:ILE:HG23 | 7 | 0.21 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 1 | 0.21 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 10 | 0.21 |
| (2,434) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HG2 | 3 | 0.21 |
| (2,434) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HG2 | 4 | 0.21 |
| (2,434) | 1:65:A:LYS:HE3 | 1:65:A:LYS:HG2 | 17 | 0.21 |
| (2,405) | 1:82:A:ILE:HG21 | 1:72:A:GLU:HG3 | 12 | 0.21 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 4 | 0.21 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 11 | 0.21 |
| (2,298) | 1:47:A:ILE:HG23 | 1:24:A:LYS:HB3 | 2 | 0.21 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 20 | 0.21 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB3 | 1 | 0.21 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB3 | 3 | 0.21 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB3 | 4 | 0.21 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 8 | 0.21 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 20 | 0.21 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 3 | 0.21 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 6 | 0.21 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 7 | 0.21 |
| (2,228) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA3 | 9 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 9 | 0.21 |
| (2,152) | 1:51:A:GLN:HE22 | 1:60:A:ILE:HA | 12 | 0.21 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 20 | 0.21 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 19 | 0.21 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 9 | 0.21 |
| (2,67) | 1:15:A:LYS:HB2 | 1:15:A:LYS:HA | 17 | 0.21 |
| (2,57) | 1:86:A:PRO:HG3 | 1:85:A:THR:HA | 9 | 0.21 |
| (2,37) | 1:68:A:PRO:HB2 | 1:87:A:ILE:HD11 | 12 | 0.21 |
| (2,29) | 1:69:A:THR:HG21 | 1:84:A:CYS:HB2 | 10 | 0.21 |
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD23 | 7 | 0.21 |
| (2,1216) | 1:46:A:ALA:HB3 | 1:83:A:ASN:H | 10 | 0.2 |
| (2,1210) | 1:46:A:ALA:HB2 | 1:26:A:GLN:H | 2 | 0.2 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 5 | 0.2 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 8 | 0.2 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 10 | 0.2 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 18 | 0.2 |
| (2,1199) | 1:56:A:ILE:HG12 | 1:57:A:GLY:H | 8 | 0.2 |
| (2,1199) | 1:56:A:ILE:HG12 | 1:57:A:GLY:H | 9 | 0.2 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 17 | 0.2 |
| (2,1154) | 1:73:A:ASP:HA | 1:32:A:GLU:H | 1 | 0.2 |
| (2,1124) | 1:41:A:VAL:HG23 | 1:44:A:GLN:HE22 | 9 | 0.2 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 4 | 0.2 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 12 | 0.2 |
| (2,1028) | 1:11:A:CYS:HA | 1:12:A:ASN:HD21 | 13 | 0.2 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 14 | 0.2 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 8 | 0.2 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 20 | 0.2 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD11 | 19 | 0.2 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 6 | 0.2 |
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 2 | 0.2 |
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 12 | 0.2 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 18 | 0.2 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG22 | 5 | 0.2 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG22 | 19 | 0.2 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 6 | 0.2 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 19 | 0.2 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 1 | 0.2 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 2 | 0.2 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 13 | 0.2 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 15 | 0.2 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 3 | 0.2 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD11 | 15 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG21 | 6 | 0.2 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG22 | 4 | 0.2 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG21 | 8 | 0.2 |
| (2,484) | 1:87:A:ILE:HG21 | 1:88:A:PRO:HD2 | 11 | 0.2 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 12 | 0.2 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 8 | 0.2 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 10 | 0.2 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD11 | 18 | 0.2 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 6 | 0.2 |
| (2,238) | 1:10:A:SER:HB3 | 1:87:A:ILE:HG23 | 19 | 0.2 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 19 | 0.2 |
| (2,228) | 1:74:A:VAL:HG22 | 1:81:A:GLY:HA3 | 2 | 0.2 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 4 | 0.2 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 17 | 0.2 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 20 | 0.2 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 1 | 0.2 |
| (2,186) | 1:68:A:PRO:HG2 | 1:67:A:THR:HA | 7 | 0.2 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 2 | 0.2 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 8 | 0.2 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 10 | 0.2 |
| (2,124) | 1:86:A:PRO:HG3 | 1:86:A:PRO:HA | 9 | 0.2 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG23 | 12 | 0.2 |
| (2,75) | 1:87:A:ILE:HG12 | 1:68:A:PRO:HB3 | 19 | 0.2 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 8 | 0.19 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 17 | 0.19 |
| (2,1266) | 1:16:A:LEU:HD11 | 1:4:A:TRP:H | 5 | 0.19 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 9 | 0.19 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 16 | 0.19 |
| (2,1199) | 1:56:A:ILE:HG12 | 1:57:A:GLY:H | 10 | 0.19 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 18 | 0.19 |
| (2,1131) | 1:23:A:LYS:HG3 | 1:22:A:ASN:H | 20 | 0.19 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 13 | 0.19 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 8 | 0.19 |
| (2,1076) | 1:29:A:THR:H | 1:28:A:SER:HA | 16 | 0.19 |
| (2,1068) | 1:47:A:ILE:HG22 | 1:21:A:THR:H | 4 | 0.19 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 1 | 0.19 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 4 | 0.19 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 5 | 0.19 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 6 | 0.19 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 9 | 0.19 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 18 | 0.19 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 10 | 0.19 |
| (2,885) | 1:47:A:ILE:HD11 | 1:47:A:ILE:HA | 19 | 0.19 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 8 | 0.19 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG21 | 13 | 0.19 |
| (2,809) | 1:42:A:LEU:H | 1:42:A:LEU:HG | 8 | 0.19 |
| (2,790) | 1:60:A:ILE:HD12 | 1:68:A:PRO:HA | 1 | 0.19 |
| (2,769) | 1:74:A:VAL:HG23 | 1:78:A:GLY:HA2 | 2 | 0.19 |
| (2,769) | 1:74:A:VAL:HG22 | 1:78:A:GLY:HA2 | 11 | 0.19 |
| (2,769) | 1:74:A:VAL:HG21 | 1:78:A:GLY:HA2 | 12 | 0.19 |
| (2,720) | 1:82:A:ILE:HG23 | 1:44:A:GLN:HA | 4 | 0.19 |
| (2,609) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HG2 | 3 | 0.19 |
| (2,600) | 1:47:A:ILE:HD12 | 1:21:A:THR:HB | 9 | 0.19 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 16 | 0.19 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 9 | 0.19 |
| (2,537) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HA | 12 | 0.19 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG22 | 5 | 0.19 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 9 | 0.19 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG21 | 11 | 0.19 |
| (2,430) | 1:63:A:GLU:H | 1:62:A:ASP:HB3 | 20 | 0.19 |
| (2,416) | 1:67:A:THR:HG21 | 1:86:A:PRO:HG3 | 11 | 0.19 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD11 | 16 | 0.19 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB2 | 8 | 0.19 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 14 | 0.19 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 10 | 0.19 |
| (2,205) | 1:74:A:VAL:HG22 | 1:15:A:LYS:HE3 | 12 | 0.19 |
| (2,183) | 1:23:A:LYS:HG3 | 1:20:A:ASP:HB2 | 8 | 0.19 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 6 | 0.19 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG23 | 16 | 0.19 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG21 | 19 | 0.19 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 6 | 0.19 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 10 | 0.19 |
| (2,142) | 1:27:A:LYS:HG2 | 1:27:A:LYS:HE3 | 19 | 0.19 |
| (2,99) | 1:58:A:ILE:HG22 | 1:58:A:ILE:HA | 3 | 0.19 |
| (2,99) | 1:58:A:ILE:HG22 | 1:58:A:ILE:HA | 8 | 0.19 |
| (2,99) | 1:58:A:ILE:HG23 | 1:58:A:ILE:HA | 11 | 0.19 |
| (2,57) | 1:86:A:PRO:HG3 | 1:85:A:THR:HA | 14 | 0.19 |
| (2,39) | 1:69:A:THR:H | 1:87:A:ILE:HD11 | 19 | 0.19 |
| (2,7) | 1:12:A:ASN:HB2 | 1:12:A:ASN:HA | 11 | 0.19 |
| (1,27) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 5 | 0.19 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 3 | 0.19 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 11 | 0.19 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 20 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3) | 1:35:A:LEU:HB3 | 1:35:A:LEU:HD23 | 1 | 0.19 |
| (2,1216) | 1:46:A:ALA:HB2 | 1:83:A:ASN:H | 11 | 0.18 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 3 | 0.18 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 12 | 0.18 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 13 | 0.18 |
| (2,1124) | 1:41:A:VAL:HG23 | 1:44:A:GLN:HE22 | 3 | 0.18 |
| (2,1078) | 1:29:A:THR:HG23 | 1:29:A:THR:H | 18 | 0.18 |
| (2,1072) | 1:31:A:GLU:H | 1:31:A:GLU:HG2 | 12 | 0.18 |
| (2,1044) | 1:47:A:ILE:HD12 | 1:19:A:CYS:H | 16 | 0.18 |
| (2,1032) | 1:87:A:ILE:HG22 | 1:10:A:SER:H | 1 | 0.18 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 18 | 0.18 |
| (2,966) | 1:43:A:ASP:HB3 | 1:42:A:LEU:H | 9 | 0.18 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 5 | 0.18 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD11 | 12 | 0.18 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD12 | 20 | 0.18 |
| (2,885) | 1:47:A:ILE:HD12 | 1:47:A:ILE:HA | 14 | 0.18 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 8 | 0.18 |
| (2,871) | 1:67:A:THR:H | 1:67:A:THR:HG23 | 10 | 0.18 |
| (2,857) | 1:90:A:ILE:HG12 | 1:88:A:PRO:HG3 | 9 | 0.18 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG22 | 12 | 0.18 |
| (2,821) | 1:11:A:CYS:H | 1:10:A:SER:HB3 | 9 | 0.18 |
| (2,821) | 1:11:A:CYS:H | 1:10:A:SER:HB3 | 10 | 0.18 |
| (2,819) | 1:35:A:LEU:H | 1:35:A:LEU:HG | 17 | 0.18 |
| (2,816) | 1:15:A:LYS:HB2 | 1:71:A:CYS:HB3 | 5 | 0.18 |
| (2,809) | 1:42:A:LEU:H | 1:42:A:LEU:HG | 5 | 0.18 |
| (2,769) | 1:74:A:VAL:HG22 | 1:78:A:GLY:HA2 | 3 | 0.18 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 2 | 0.18 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 12 | 0.18 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 19 | 0.18 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 9 | 0.18 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 1 | 0.18 |
| (2,541) | 1:87:A:ILE:HG21 | 1:10:A:SER:HA | 11 | 0.18 |
| (2,516) | 1:31:A:GLU:HA | 1:31:A:GLU:HB3 | 9 | 0.18 |
| (2,516) | 1:31:A:GLU:HA | 1:31:A:GLU:HB3 | 12 | 0.18 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG21 | 13 | 0.18 |
| (2,475) | 1:61:A:GLU:HG2 | 1:60:A:ILE:HG23 | 9 | 0.18 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG22 | 13 | 0.18 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG22 | 17 | 0.18 |
| (2,405) | 1:82:A:ILE:HG22 | 1:72:A:GLU:HG3 | 3 | 0.18 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 9 | 0.18 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 14 | 0.18 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD13 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,328) | 1:72:A:GLU:HG2 | 1:83:A:ASN:HB2 | 18 | 0.18 |
| (2,260) | 1:69:A:THR:HG21 | 1:19:A:CYS:HB3 | 14 | 0.18 |
| (2,244) | 1:62:A:ASP:HB3 | 1:58:A:ILE:HG23 | 1 | 0.18 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG21 | 11 | 0.18 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG21 | 10 | 0.18 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 12 | 0.18 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 15 | 0.18 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 19 | 0.18 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 9 | 0.18 |
| (2,99) | 1:58:A:ILE:HG22 | 1:58:A:ILE:HA | 19 | 0.18 |
| (2,57) | 1:86:A:PRO:HG3 | 1:85:A:THR:HA | 5 | 0.18 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 8 | 0.18 |
| (2,38) | 1:10:A:SER:HB3 | 1:87:A:ILE:HD11 | 9 | 0.18 |
| (2,29) | 1:69:A:THR:HG21 | 1:84:A:CYS:HB2 | 5 | 0.18 |
| (2,29) | 1:69:A:THR:HG23 | 1:84:A:CYS:HB2 | 19 | 0.18 |
| (2,29) | 1:69:A:THR:HG21 | 1:84:A:CYS:HB2 | 20 | 0.18 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 1 | 0.18 |
| (2,1292) | 1:67:A:THR:HG21 | 1:21:A:THR:H | 10 | 0.17 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 3 | 0.17 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 4 | 0.17 |
| (2,1221) | 1:27:A:LYS:H | 1:27:A:LYS:HB2 | 16 | 0.17 |
| (2,1213) | 1:45:A:VAL:HG23 | 1:83:A:ASN:H | 19 | 0.17 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 6 | 0.17 |
| (2,1183) | 1:68:A:PRO:HB3 | 1:87:A:ILE:H | 9 | 0.17 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 10 | 0.17 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 18 | 0.17 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 19 | 0.17 |
| (2,1143) | 1:25:A:VAL:HG23 | 1:24:A:LYS:H | 1 | 0.17 |
| (2,1122) | 1:82:A:ILE:HD13 | 1:44:A:GLN:HE22 | 19 | 0.17 |
| (2,1119) | 1:80:A:VAL:HG13 | 1:80:A:VAL:H | 1 | 0.17 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 14 | 0.17 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 16 | 0.17 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 17 | 0.17 |
| (2,1068) | 1:47:A:ILE:HG21 | 1:21:A:THR:H | 2 | 0.17 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 3 | 0.17 |
| (2,1032) | 1:87:A:ILE:HG22 | 1:10:A:SER:H | 11 | 0.17 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 12 | 0.17 |
| (2,923) | 1:21:A:THR:HG22 | 1:67:A:THR:HB | 17 | 0.17 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 14 | 0.17 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD11 | 20 | 0.17 |
| (2,885) | 1:47:A:ILE:HD13 | 1:47:A:ILE:HA | 13 | 0.17 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 16 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 9 | 0.17 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 11 | 0.17 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG21 | 4 | 0.17 |
| (2,831) | 1:49:A:CYS:H | 1:48:A:GLN:HB2 | 5 | 0.17 |
| (2,825) | 1:8:A:THR:HG23 | 1:10:A:SER:HB3 | 1 | 0.17 |
| (2,809) | 1:42:A:LEU:H | 1:42:A:LEU:HG | 6 | 0.17 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 6 | 0.17 |
| (2,626) | 1:52:A:ILE:HB | 1:64:A:CYS:HB2 | 2 | 0.17 |
| (2,621) | 1:66:A:ASN:HD21 | 1:18:A:CYS:HB2 | 19 | 0.17 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 5 | 0.17 |
| (2,610) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HB3 | 14 | 0.17 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 10 | 0.17 |
| (2,544) | 1:79:A:LEU:HA | 1:79:A:LEU:HD22 | 10 | 0.17 |
| (2,541) | 1:87:A:ILE:HG22 | 1:10:A:SER:HA | 17 | 0.17 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG23 | 10 | 0.17 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG23 | 2 | 0.17 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG21 | 14 | 0.17 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG22 | 5 | 0.17 |
| (2,452) | 1:72:A:GLU:H | 1:72:A:GLU:HB3 | 16 | 0.17 |
| (2,416) | 1:67:A:THR:HG23 | 1:86:A:PRO:HG3 | 14 | 0.17 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 11 | 0.17 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 20 | 0.17 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 8 | 0.17 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD11 | 12 | 0.17 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 13 | 0.17 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 19 | 0.17 |
| (2,328) | 1:72:A:GLU:HG2 | 1:83:A:ASN:HB2 | 9 | 0.17 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 14 | 0.17 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 19 | 0.17 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 4 | 0.17 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 15 | 0.17 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 5 | 0.17 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 14 | 0.17 |
| (2,109) | 1:13:A:THR:HG22 | 1:12:A:ASN:HB2 | 17 | 0.17 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 4 | 0.17 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 10 | 0.17 |
| (1,27) | 1:48:A:GLN:HG2 | 1:48:A:GLN:H | 16 | 0.17 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 6 | 0.17 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 10 | 0.17 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 16 | 0.16 |
| (2,1216) | 1:46:A:ALA:HB2 | 1:83:A:ASN:H | 1 | 0.16 |
| (2,1216) | 1:46:A:ALA:HB2 | 1:83:A:ASN:H | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 2 | 0.16 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 7 | 0.16 |
| (2,1143) | 1:25:A:VAL:HG23 | 1:24:A:LYS:H | 16 | 0.16 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 10 | 0.16 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 11 | 0.16 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 11 | 0.16 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 2 | 0.16 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 12 | 0.16 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 15 | 0.16 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 19 | 0.16 |
| (2,923) | 1:21:A:THR:HG22 | 1:67:A:THR:HB | 1 | 0.16 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 4 | 0.16 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 7 | 0.16 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 13 | 0.16 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 16 | 0.16 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 8 | 0.16 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 2 | 0.16 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 2 | 0.16 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 5 | 0.16 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 3 | 0.16 |
| (2,889) | 1:47:A:ILE:HD12 | 1:19:A:CYS:HA | 18 | 0.16 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 1 | 0.16 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 13 | 0.16 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 12 | 0.16 |
| (2,819) | 1:35:A:LEU:H | 1:35:A:LEU:HG | 3 | 0.16 |
| (2,819) | 1:35:A:LEU:H | 1:35:A:LEU:HG | 12 | 0.16 |
| (2,815) | 1:17:A:ALA:HB1 | 1:71:A:CYS:HB3 | 4 | 0.16 |
| (2,758) | 1:76:A:ASP:H | 1:75:A:GLU:HG3 | 8 | 0.16 |
| (2,719) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB3 | 9 | 0.16 |
| (2,630) | 1:52:A:ILE:HD12 | 1:64:A:CYS:HB3 | 6 | 0.16 |
| (2,630) | 1:52:A:ILE:HD11 | 1:64:A:CYS:HB3 | 20 | 0.16 |
| (2,568) | 1:25:A:VAL:HG23 | 1:48:A:GLN:HB2 | 9 | 0.16 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 3 | 0.16 |
| (2,558) | 1:49:A:CYS:H | 1:49:A:CYS:HB3 | 17 | 0.16 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD13 | 9 | 0.16 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG22 | 2 | 0.16 |
| (2,484) | 1:87:A:ILE:HG23 | 1:88:A:PRO:HD2 | 14 | 0.16 |
| (2,484) | 1:87:A:ILE:HG21 | 1:88:A:PRO:HD2 | 16 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG21 | 8 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 10 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG21 | 16 | 0.16 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 18 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 20 | 0.16 |
| (2,423) | 1:54:A:LEU:H | 1:54:A:LEU:HD13 | 2 | 0.16 |
| (2,416) | 1:67:A:THR:HG21 | 1:86:A:PRO:HG3 | 6 | 0.16 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 19 | 0.16 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD13 | 6 | 0.16 |
| (2,293) | 1:4:A:TRP:HB3 | 1:16:A:LEU:HB3 | 4 | 0.16 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 18 | 0.16 |
| (2,257) | 1:59:A:ALA:H | 1:58:A:ILE:HB | 4 | 0.16 |
| (2,228) | 1:74:A:VAL:HG23 | 1:81:A:GLY:HA3 | 13 | 0.16 |
| (2,183) | 1:23:A:LYS:HG3 | 1:20:A:ASP:HB2 | 3 | 0.16 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 2 | 0.16 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 16 | 0.16 |
| (2,154) | 1:23:A:LYS:HG3 | 1:23:A:LYS:HE3 | 17 | 0.16 |
| (2,129) | 1:79:A:LEU:HG | 1:76:A:ASP:HB2 | 17 | 0.16 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 13 | 0.16 |
| (2,120) | 1:48:A:GLN:H | 1:47:A:ILE:HG21 | 13 | 0.16 |
| (2,109) | 1:13:A:THR:HG21 | 1:12:A:ASN:HB2 | 20 | 0.16 |
| (2,108) | 1:86:A:PRO:HA | 1:67:A:THR:HG23 | 11 | 0.16 |
| (1,7) | 1:41:A:VAL:HG12 | 1:40:A:ASP:HB3 | 11 | 0.16 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 17 | 0.16 |
| (2,1209) | 1:26:A:GLN:H | 1:25:A:VAL:HB | 19 | 0.15 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 1 | 0.15 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 2 | 0.15 |
| (2,1116) | 1:22:A:ASN:HA | 1:22:A:ASN:HD21 | 5 | 0.15 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 6 | 0.15 |
| (2,1077) | 1:28:A:SER:HB2 | 1:29:A:THR:H | 12 | 0.15 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 8 | 0.15 |
| (2,1044) | 1:47:A:ILE:HD13 | 1:19:A:CYS:H | 18 | 0.15 |
| (2,1044) | 1:47:A:ILE:HD12 | 1:19:A:CYS:H | 20 | 0.15 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 10 | 0.15 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 20 | 0.15 |
| (2,1029) | 1:13:A:THR:HG22 | 1:12:A:ASN:HD21 | 17 | 0.15 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 3 | 0.15 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 19 | 0.15 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 10 | 0.15 |
| (2,939) | 1:79:A:LEU:HB2 | 1:49:A:CYS:H | 4 | 0.15 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 20 | 0.15 |
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 2 | 0.15 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 11 | 0.15 |
| (2,923) | 1:21:A:THR:HG21 | 1:67:A:THR:HB | 18 | 0.15 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 4 | 0.15 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 19 | 0.15 |
| (2,898) | 1:90:A:ILE:H | 1:88:A:PRO:HD2 | 16 | 0.15 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 2 | 0.15 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 10 | 0.15 |
| (2,856) | 1:90:A:ILE:HD11 | 1:88:A:PRO:HG3 | 15 | 0.15 |
| (2,815) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB3 | 20 | 0.15 |
| (2,758) | 1:76:A:ASP:H | 1:75:A:GLU:HG3 | 3 | 0.15 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 13 | 0.15 |
| (2,744) | 1:48:A:GLN:H | 1:48:A:GLN:HG3 | 13 | 0.15 |
| (2,720) | 1:82:A:ILE:HG21 | 1:44:A:GLN:HA | 3 | 0.15 |
| (2,706) | 1:83:A:ASN:H | 1:45:A:VAL:HB | 4 | 0.15 |
| (2,706) | 1:83:A:ASN:H | 1:45:A:VAL:HB | 8 | 0.15 |
| (2,706) | 1:83:A:ASN:H | 1:45:A:VAL:HB | 11 | 0.15 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 10 | 0.15 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 3 | 0.15 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 6 | 0.15 |
| (2,543) | 1:79:A:LEU:HD23 | 1:50:A:THR:HA | 9 | 0.15 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD11 | 3 | 0.15 |
| (2,532) | 1:46:A:ALA:HA | 1:82:A:ILE:HD12 | 16 | 0.15 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG21 | 3 | 0.15 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 3 | 0.15 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG21 | 6 | 0.15 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 20 | 0.15 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 7 | 0.15 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 17 | 0.15 |
| (2,404) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HG2 | 11 | 0.15 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD11 | 2 | 0.15 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 10 | 0.15 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 15 | 0.15 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD13 | 20 | 0.15 |
| (2,328) | 1:72:A:GLU:HG2 | 1:83:A:ASN:HB2 | 6 | 0.15 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 14 | 0.15 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 1 | 0.15 |
| (2,228) | 1:74:A:VAL:HG21 | 1:81:A:GLY:HA3 | 11 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 2 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 3 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 10 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 11 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 14 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 17 | 0.15 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 18 | 0.15 |
| (2,174) | 1:83:A:ASN:H | 1:82:A:ILE:HG22 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 14 | 0.15 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 15 | 0.15 |
| (2,72) | 1:55:A:LEU:HA | 1:55:A:LEU:HG | 12 | 0.15 |
| (2,57) | 1:86:A:PRO:HG3 | 1:85:A:THR:HA | 13 | 0.15 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 10 | 0.15 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 20 | 0.15 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 5 | 0.15 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 6 | 0.15 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 7 | 0.15 |
| (2,7) | 1:12:A:ASN:HB2 | 1:12:A:ASN:HA | 4 | 0.15 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 12 | 0.15 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 13 | 0.15 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 14 | 0.15 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 15 | 0.15 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 16 | 0.15 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 18 | 0.15 |
| (2,1292) | 1:67:A:THR:HG22 | 1:21:A:THR:H | 17 | 0.14 |
| (2,1290) | 1:60:A:ILE:HD11 | 1:19:A:CYS:H | 7 | 0.14 |
| (2,1290) | 1:60:A:ILE:HD12 | 1:19:A:CYS:H | 14 | 0.14 |
| (2,1274) | 1:23:A:LYS:HE3 | 1:24:A:LYS:H | 10 | 0.14 |
| (2,1255) | 1:82:A:ILE:HD11 | 1:44:A:GLN:HE21 | 9 | 0.14 |
| (2,1216) | 1:46:A:ALA:HB2 | 1:83:A:ASN:H | 18 | 0.14 |
| (2,1210) | 1:46:A:ALA:HB2 | 1:26:A:GLN:H | 16 | 0.14 |
| (2,1205) | 1:35:A:LEU:HB3 | 1:36:A:LEU:H | 6 | 0.14 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 15 | 0.14 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 20 | 0.14 |
| (2,1199) | 1:56:A:ILE:HG12 | 1:57:A:GLY:H | 19 | 0.14 |
| (2,1189) | 1:54:A:LEU:H | 1:54:A:LEU:HA | 4 | 0.14 |
| (2,1189) | 1:54:A:LEU:H | 1:54:A:LEU:HA | 13 | 0.14 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 7 | 0.14 |
| (2,1159) | 1:47:A:ILE:HG21 | 1:46:A:ALA:H | 19 | 0.14 |
| (2,1119) | 1:80:A:VAL:HG11 | 1:80:A:VAL:H | 4 | 0.14 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 7 | 0.14 |
| (2,1115) | 1:75:A:GLU:HB2 | 1:76:A:ASP:H | 10 | 0.14 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 19 | 0.14 |
| (2,1083) | 1:26:A:GLN:HB2 | 1:26:A:GLN:HE21 | 15 | 0.14 |
| (2,1068) | 1:47:A:ILE:HG21 | 1:21:A:THR:H | 12 | 0.14 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 7 | 0.14 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 11 | 0.14 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 4 | 0.14 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 15 | 0.14 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 15 | 0.14 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 18 | 0.14 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 19 | 0.14 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 5 | 0.14 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 1 | 0.14 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 8 | 0.14 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 12 | 0.14 |
| (2,919) | 1:67:A:THR:H | 1:68:A:PRO:HD2 | 20 | 0.14 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 7 | 0.14 |
| (2,889) | 1:47:A:ILE:HD13 | 1:19:A:CYS:HA | 6 | 0.14 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 15 | 0.14 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 5 | 0.14 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 9 | 0.14 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 10 | 0.14 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 15 | 0.14 |
| (2,877) | 1:80:A:VAL:H | 1:78:A:GLY:HA3 | 10 | 0.14 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 5 | 0.14 |
| (2,866) | 1:70:A:CYS:H | 1:87:A:ILE:HD12 | 2 | 0.14 |
| (2,809) | 1:42:A:LEU:H | 1:42:A:LEU:HG | 19 | 0.14 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 9 | 0.14 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 13 | 0.14 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 14 | 0.14 |
| (2,713) | 1:17:A:ALA:HB3 | 1:71:A:CYS:HB2 | 3 | 0.14 |
| (2,706) | 1:83:A:ASN:H | 1:45:A:VAL:HB | 20 | 0.14 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 14 | 0.14 |
| (2,681) | 1:60:A:ILE:HD11 | 1:18:A:CYS:HB3 | 7 | 0.14 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 12 | 0.14 |
| (2,626) | 1:52:A:ILE:HB | 1:64:A:CYS:HB2 | 19 | 0.14 |
| (2,599) | 1:47:A:ILE:HG22 | 1:21:A:THR:HB | 5 | 0.14 |
| (2,589) | 1:15:A:LYS:H | 1:14:A:GLY:HA2 | 13 | 0.14 |
| (2,562) | 1:53:A:PRO:HD2 | 1:52:A:ILE:HB | 20 | 0.14 |
| (2,551) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB3 | 8 | 0.14 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 4 | 0.14 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD21 | 14 | 0.14 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG21 | 4 | 0.14 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG23 | 6 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 1 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 7 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 13 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 16 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 17 | 0.14 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 18 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 19 | 0.14 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG22 | 4 | 0.14 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 7 | 0.14 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 14 | 0.14 |
| (2,422) | 1:79:A:LEU:HD12 | 1:79:A:LEU:HG | 1 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 3 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 4 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 7 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 9 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 14 | 0.14 |
| (2,422) | 1:79:A:LEU:HD12 | 1:79:A:LEU:HG | 15 | 0.14 |
| (2,422) | 1:79:A:LEU:HD12 | 1:79:A:LEU:HG | 16 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 18 | 0.14 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 20 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 1 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 2 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 3 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 5 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 6 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 8 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 10 | 0.14 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 20 | 0.14 |
| (2,409) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HB3 | 9 | 0.14 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 2 | 0.14 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 10 | 0.14 |
| (2,387) | 1:66:A:ASN:HD21 | 1:66:A:ASN:HA | 11 | 0.14 |
| (2,372) | 1:79:A:LEU:H | 1:79:A:LEU:HG | 9 | 0.14 |
| (2,270) | 1:47:A:ILE:H | 1:46:A:ALA:HB1 | 12 | 0.14 |
| (2,223) | 1:77:A:ASP:HA | 1:77:A:ASP:HB3 | 15 | 0.14 |
| (2,198) | 1:51:A:GLN:HB2 | 1:51:A:GLN:HA | 2 | 0.14 |
| (2,194) | 1:24:A:LYS:HA | 1:47:A:ILE:HG21 | 1 | 0.14 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 20 | 0.14 |
| (2,180) | 1:69:A:THR:HG22 | 1:86:A:PRO:HB2 | 9 | 0.14 |
| (2,174) | 1:83:A:ASN:H | 1:82:A:ILE:HG23 | 16 | 0.14 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 18 | 0.14 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 7 | 0.14 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 16 | 0.14 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 14 | 0.14 |
| (2,130) | 1:79:A:LEU:HB3 | 1:76:A:ASP:HB2 | 4 | 0.14 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 9 | 0.14 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 12 | 0.14 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 18 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 2 | 0.14 |
| (2,1292) | 1:67:A:THR:HG23 | 1:21:A:THR:H | 19 | 0.13 |
| (2,1216) | 1:46:A:ALA:HB3 | 1:83:A:ASN:H | 19 | 0.13 |
| (2,1209) | 1:26:A:GLN:H | 1:25:A:VAL:HB | 2 | 0.13 |
| (2,1209) | 1:26:A:GLN:H | 1:25:A:VAL:HB | 9 | 0.13 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 11 | 0.13 |
| (2,1180) | 1:50:A:THR:HG22 | 1:51:A:GLN:H | 17 | 0.13 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 12 | 0.13 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 19 | 0.13 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 5 | 0.13 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 16 | 0.13 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 2 | 0.13 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 6 | 0.13 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 14 | 0.13 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 16 | 0.13 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 17 | 0.13 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 3 | 0.13 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 8 | 0.13 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 1 | 0.13 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 3 | 0.13 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 13 | 0.13 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 14 | 0.13 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 11 | 0.13 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 13 | 0.13 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 19 | 0.13 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 20 | 0.13 |
| (2,898) | 1:90:A:ILE:H | 1:88:A:PRO:HD2 | 19 | 0.13 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 9 | 0.13 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 7 | 0.13 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 16 | 0.13 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 18 | 0.13 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 1 | 0.13 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 3 | 0.13 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 8 | 0.13 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 14 | 0.13 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 19 | 0.13 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 10 | 0.13 |
| (2,857) | 1:90:A:ILE:HG12 | 1:88:A:PRO:HG3 | 4 | 0.13 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG23 | 11 | 0.13 |
| (2,830) | 1:72:A:GLU:H | 1:72:A:GLU:HG3 | 13 | 0.13 |
| (2,790) | 1:60:A:ILE:HD12 | 1:68:A:PRO:HA | 11 | 0.13 |
| (2,769) | 1:74:A:VAL:HG21 | 1:78:A:GLY:HA2 | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 1 | 0.13 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 11 | 0.13 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 15 | 0.13 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 19 | 0.13 |
| (2,720) | 1:82:A:ILE:HG22 | 1:44:A:GLN:HA | 18 | 0.13 |
| (2,706) | 1:83:A:ASN:H | 1:45:A:VAL:HB | 10 | 0.13 |
| (2,703) | 1:60:A:ILE:HG12 | 1:18:A:CYS:HB3 | 12 | 0.13 |
| (2,694) | 1:78:A:GLY:HA3 | 1:74:A:VAL:HB | 5 | 0.13 |
| (2,694) | 1:78:A:GLY:HA3 | 1:74:A:VAL:HB | 12 | 0.13 |
| (2,603) | 1:16:A:LEU:HD12 | 1:70:A:CYS:HA | 14 | 0.13 |
| (2,589) | 1:15:A:LYS:H | 1:14:A:GLY:HA2 | 9 | 0.13 |
| (2,554) | 1:49:A:CYS:HB2 | 1:17:A:ALA:HB3 | 4 | 0.13 |
| (2,551) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB3 | 3 | 0.13 |
| (2,551) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB3 | 9 | 0.13 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG21 | 5 | 0.13 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG23 | 12 | 0.13 |
| (2,506) | 1:59:A:ALA:HA | 1:60:A:ILE:HG22 | 13 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 2 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 3 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 4 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 6 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 8 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 9 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 10 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 11 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 12 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 15 | 0.13 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 20 | 0.13 |
| (2,469) | 1:88:A:PRO:HD3 | 1:87:A:ILE:HG23 | 15 | 0.13 |
| (2,453) | 1:73:A:ASP:H | 1:72:A:GLU:HB3 | 18 | 0.13 |
| (2,437) | 1:26:A:GLN:H | 1:26:A:GLN:HG2 | 15 | 0.13 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 2 | 0.13 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 5 | 0.13 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 8 | 0.13 |
| (2,422) | 1:79:A:LEU:HD13 | 1:79:A:LEU:HG | 11 | 0.13 |
| (2,422) | 1:79:A:LEU:HD12 | 1:79:A:LEU:HG | 13 | 0.13 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 19 | 0.13 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD13 | 3 | 0.13 |
| (2,420) | 1:76:A:ASP:HB3 | 1:79:A:LEU:HD13 | 7 | 0.13 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 4 | 0.13 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 16 | 0.13 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,409) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HB3 | 5 | 0.13 |
| (2,409) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HB3 | 14 | 0.13 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 8 | 0.13 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 12 | 0.13 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 9 | 0.13 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 14 | 0.13 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 1 | 0.13 |
| (2,338) | 1:16:A:LEU:HA | 1:16:A:LEU:HD12 | 5 | 0.13 |
| (2,183) | 1:23:A:LYS:HG3 | 1:20:A:ASP:HB2 | 1 | 0.13 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 12 | 0.13 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 17 | 0.13 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG22 | 9 | 0.13 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG22 | 11 | 0.13 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 16 | 0.13 |
| (2,152) | 1:51:A:GLN:HE22 | 1:60:A:ILE:HA | 8 | 0.13 |
| (2,152) | 1:51:A:GLN:HE22 | 1:60:A:ILE:HA | 13 | 0.13 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 4 | 0.13 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 7 | 0.13 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 9 | 0.13 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 4 | 0.13 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 9 | 0.13 |
| (2,1280) | 1:39:A:GLY:HA3 | 1:41:A:VAL:H | 16 | 0.12 |
| (2,1258) | 1:18:A:CYS:H | 1:4:A:TRP:HE1 | 19 | 0.12 |
| (2,1216) | 1:46:A:ALA:HB1 | 1:83:A:ASN:H | 8 | 0.12 |
| (2,1186) | 1:87:A:ILE:H | 1:88:A:PRO:HD2 | 11 | 0.12 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 3 | 0.12 |
| (2,1182) | 1:51:A:GLN:H | 1:51:A:GLN:HG3 | 15 | 0.12 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 13 | 0.12 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 18 | 0.12 |
| (2,1124) | 1:41:A:VAL:HG21 | 1:44:A:GLN:HE22 | 18 | 0.12 |
| (2,1119) | 1:80:A:VAL:HG11 | 1:80:A:VAL:H | 17 | 0.12 |
| (2,1119) | 1:80:A:VAL:HG13 | 1:80:A:VAL:H | 19 | 0.12 |
| (2,1068) | 1:47:A:ILE:HG22 | 1:21:A:THR:H | 13 | 0.12 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 2 | 0.12 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 9 | 0.12 |
| (2,1024) | 1:85:A:THR:HG23 | 1:85:A:THR:H | 14 | 0.12 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 4 | 0.12 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 8 | 0.12 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 13 | 0.12 |
| (2,1020) | 1:41:A:VAL:HB | 1:44:A:GLN:H | 17 | 0.12 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 5 | 0.12 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 12 | 0.12 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 20 | 0.12 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 17 | 0.12 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 11 | 0.12 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 12 | 0.12 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 2 | 0.12 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 12 | 0.12 |
| (2,953) | 1:90:A:ILE:H | 1:89:A:LEU:HA | 7 | 0.12 |
| (2,940) | 1:79:A:LEU:HD22 | 1:49:A:CYS:H | 11 | 0.12 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 12 | 0.12 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 16 | 0.12 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD13 | 10 | 0.12 |
| (2,921) | 1:24:A:LYS:H | 1:23:A:LYS:HG3 | 11 | 0.12 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 10 | 0.12 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 16 | 0.12 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 17 | 0.12 |
| (2,912) | 1:61:A:GLU:H | 1:61:A:GLU:HG2 | 10 | 0.12 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 17 | 0.12 |
| (2,904) | 1:16:A:LEU:HG | 1:11:A:CYS:HB2 | 5 | 0.12 |
| (2,904) | 1:16:A:LEU:HG | 1:11:A:CYS:HB2 | 10 | 0.12 |
| (2,895) | 1:48:A:GLN:H | 1:47:A:ILE:HD11 | 16 | 0.12 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 13 | 0.12 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 11 | 0.12 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 1 | 0.12 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 6 | 0.12 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 13 | 0.12 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 16 | 0.12 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 18 | 0.12 |
| (2,853) | 1:69:A:THR:HA | 1:87:A:ILE:HG22 | 3 | 0.12 |
| (2,830) | 1:72:A:GLU:H | 1:72:A:GLU:HG3 | 11 | 0.12 |
| (2,815) | 1:17:A:ALA:HB2 | 1:71:A:CYS:HB3 | 19 | 0.12 |
| (2,809) | 1:42:A:LEU:H | 1:42:A:LEU:HG | 20 | 0.12 |
| (2,797) | 1:25:A:VAL:H | 1:24:A:LYS:HB2 | 18 | 0.12 |
| (2,769) | 1:74:A:VAL:HG21 | 1:78:A:GLY:HA2 | 17 | 0.12 |
| (2,766) | 1:68:A:PRO:HG2 | 1:61:A:GLU:HA | 18 | 0.12 |
| (2,754) | 1:5:A:GLU:H | 1:5:A:GLU:HG2 | 3 | 0.12 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 4 | 0.12 |
| (2,747) | 1:83:A:ASN:HD22 | 1:72:A:GLU:HB3 | 8 | 0.12 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 1 | 0.12 |
| (2,741) | 1:48:A:GLN:HE22 | 1:48:A:GLN:HG3 | 2 | 0.12 |
| (2,700) | 1:19:A:CYS:HB2 | 1:47:A:ILE:HG12 | 11 | 0.12 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 4 | 0.12 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 3 | 0.12 |
| (2,570) | 1:23:A:LYS:HE3 | 1:48:A:GLN:HB2 | 16 | 0.12 |
| (2,562) | 1:53:A:PRO:HD2 | 1:52:A:ILE:HB | 12 | 0.12 |
| (2,545) | 1:79:A:LEU:HB2 | 1:79:A:LEU:HD23 | 8 | 0.12 |
| (2,537) | 1:25:A:VAL:HG21 | 1:48:A:GLN:HA | 9 | 0.12 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 5 | 0.12 |
| (2,484) | 1:87:A:ILE:HG21 | 1:88:A:PRO:HD2 | 6 | 0.12 |
| (2,423) | 1:54:A:LEU:H | 1:54:A:LEU:HD11 | 20 | 0.12 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 6 | 0.12 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 10 | 0.12 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 12 | 0.12 |
| (2,422) | 1:79:A:LEU:HD11 | 1:79:A:LEU:HG | 17 | 0.12 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 14 | 0.12 |
| (2,409) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HB3 | 13 | 0.12 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 1 | 0.12 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 7 | 0.12 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 9 | 0.12 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 15 | 0.12 |
| (2,387) | 1:66:A:ASN:HD21 | 1:66:A:ASN:HA | 12 | 0.12 |
| (2,298) | 1:47:A:ILE:HG22 | 1:24:A:LYS:HB3 | 20 | 0.12 |
| (2,277) | 1:23:A:LYS:HA | 1:23:A:LYS:HG3 | 15 | 0.12 |
| (2,257) | 1:59:A:ALA:H | 1:58:A:ILE:HB | 5 | 0.12 |
| (2,245) | 1:63:A:GLU:HG2 | 1:58:A:ILE:HG23 | 8 | 0.12 |
| (2,230) | 1:74:A:VAL:HA | 1:81:A:GLY:HA3 | 18 | 0.12 |
| (2,218) | 1:49:A:CYS:HB3 | 1:79:A:LEU:HA | 5 | 0.12 |
| (2,209) | 1:68:A:PRO:HB2 | 1:68:A:PRO:HD2 | 8 | 0.12 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 8 | 0.12 |
| (2,182) | 1:87:A:ILE:H | 1:86:A:PRO:HB2 | 18 | 0.12 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG21 | 3 | 0.12 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG23 | 4 | 0.12 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG21 | 13 | 0.12 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG22 | 18 | 0.12 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 8 | 0.12 |
| (2,152) | 1:51:A:GLN:HE22 | 1:60:A:ILE:HA | 20 | 0.12 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 3 | 0.12 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 9 | 0.12 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 20 | 0.12 |
| (2,143) | 1:27:A:LYS:HB3 | 1:27:A:LYS:HE3 | 6 | 0.12 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 8 | 0.12 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 11 | 0.12 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 18 | 0.12 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 19 | 0.12 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 5 | 0.12 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 5 | 0.12 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 8 | 0.12 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 11 | 0.12 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 13 | 0.12 |
| (2,1286) | 1:46:A:ALA:HB2 | 1:81:A:GLY:H | 9 | 0.11 |
| (2,1278) | 1:38:A:THR:HA | 1:41:A:VAL:H | 7 | 0.11 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 4 | 0.11 |
| (2,1201) | 1:57:A:GLY:H | 1:56:A:ILE:HB | 14 | 0.11 |
| (2,1189) | 1:54:A:LEU:H | 1:54:A:LEU:HA | 16 | 0.11 |
| (2,1186) | 1:87:A:ILE:H | 1:88:A:PRO:HD2 | 16 | 0.11 |
| (2,1168) | 1:48:A:GLN:HB2 | 1:20:A:ASP:H | 14 | 0.11 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 14 | 0.11 |
| (2,1164) | 1:20:A:ASP:H | 1:19:A:CYS:HB2 | 17 | 0.11 |
| (2,1163) | 1:50:A:THR:HG21 | 1:20:A:ASP:H | 20 | 0.11 |
| (2,1144) | 1:23:A:LYS:H | 1:24:A:LYS:H | 3 | 0.11 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 6 | 0.11 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 7 | 0.11 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 16 | 0.11 |
| (2,1119) | 1:80:A:VAL:HG12 | 1:80:A:VAL:H | 12 | 0.11 |
| (2,1094) | 1:66:A:ASN:H | 1:66:A:ASN:HB3 | 12 | 0.11 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 18 | 0.11 |
| (2,1024) | 1:85:A:THR:HG23 | 1:85:A:THR:H | 1 | 0.11 |
| (2,1024) | 1:85:A:THR:HG21 | 1:85:A:THR:H | 4 | 0.11 |
| (2,1018) | 1:41:A:VAL:H | 1:40:A:ASP:HB3 | 11 | 0.11 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 3 | 0.11 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 7 | 0.11 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 11 | 0.11 |
| (2,1017) | 1:44:A:GLN:H | 1:44:A:GLN:HA | 18 | 0.11 |
| (2,994) | 1:30:A:GLY:H | 1:29:A:THR:HA | 20 | 0.11 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 3 | 0.11 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 10 | 0.11 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 15 | 0.11 |
| (2,989) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HB3 | 18 | 0.11 |
| (2,958) | 1:72:A:GLU:H | 1:72:A:GLU:HG2 | 11 | 0.11 |
| (2,939) | 1:79:A:LEU:HB2 | 1:49:A:CYS:H | 6 | 0.11 |
| (2,922) | 1:79:A:LEU:H | 1:79:A:LEU:HD12 | 16 | 0.11 |
| (2,914) | 1:23:A:LYS:HA | 1:24:A:LYS:HB2 | 3 | 0.11 |
| (2,913) | 1:61:A:GLU:H | 1:61:A:GLU:HG3 | 9 | 0.11 |
| (2,905) | 1:8:A:THR:H | 1:7:A:LYS:HD3 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,889) | 1:47:A:ILE:HD13 | 1:19:A:CYS:HA | 17 | 0.11 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 13 | 0.11 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 20 | 0.11 |
| (2,877) | 1:80:A:VAL:H | 1:78:A:GLY:HA3 | 9 | 0.11 |
| (2,856) | 1:90:A:ILE:HD13 | 1:88:A:PRO:HG3 | 8 | 0.11 |
| (2,830) | 1:72:A:GLU:H | 1:72:A:GLU:HG3 | 7 | 0.11 |
| (2,830) | 1:72:A:GLU:H | 1:72:A:GLU:HG3 | 20 | 0.11 |
| (2,720) | 1:82:A:ILE:HG23 | 1:44:A:GLN:HA | 15 | 0.11 |
| (2,712) | 1:48:A:GLN:HG3 | 1:25:A:VAL:HG23 | 11 | 0.11 |
| (2,694) | 1:78:A:GLY:HA3 | 1:74:A:VAL:HB | 3 | 0.11 |
| (2,694) | 1:78:A:GLY:HA3 | 1:74:A:VAL:HB | 4 | 0.11 |
| (2,694) | 1:78:A:GLY:HA3 | 1:74:A:VAL:HB | 16 | 0.11 |
| (2,681) | 1:60:A:ILE:HD12 | 1:18:A:CYS:HB3 | 18 | 0.11 |
| (2,665) | 1:72:A:GLU:HB3 | 1:71:A:CYS:HA | 1 | 0.11 |
| (2,626) | 1:52:A:ILE:HB | 1:64:A:CYS:HB2 | 18 | 0.11 |
| (2,609) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HG2 | 14 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 3 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 6 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 9 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 10 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 18 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 19 | 0.11 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 20 | 0.11 |
| (2,589) | 1:15:A:LYS:H | 1:14:A:GLY:HA2 | 4 | 0.11 |
| (2,589) | 1:15:A:LYS:H | 1:14:A:GLY:HA2 | 8 | 0.11 |
| (2,569) | 1:23:A:LYS:HB2 | 1:48:A:GLN:HB2 | 8 | 0.11 |
| (2,551) | 1:23:A:LYS:HB2 | 1:20:A:ASP:HB3 | 1 | 0.11 |
| (2,492) | 1:44:A:GLN:HB3 | 1:44:A:GLN:HG3 | 14 | 0.11 |
| (2,424) | 1:72:A:GLU:HG2 | 1:72:A:GLU:HA | 17 | 0.11 |
| (2,417) | 1:40:A:ASP:HB3 | 1:40:A:ASP:HA | 15 | 0.11 |
| (2,407) | 1:26:A:GLN:H | 1:26:A:GLN:HB3 | 6 | 0.11 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 1 | 0.11 |
| (2,324) | 1:21:A:THR:HA | 1:47:A:ILE:HD11 | 13 | 0.11 |
| (2,257) | 1:59:A:ALA:H | 1:58:A:ILE:HB | 10 | 0.11 |
| (2,231) | 1:46:A:ALA:HA | 1:47:A:ILE:HG22 | 6 | 0.11 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG22 | 6 | 0.11 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG23 | 15 | 0.11 |
| (2,170) | 1:82:A:ILE:HA | 1:82:A:ILE:HG22 | 17 | 0.11 |
| (2,166) | 1:36:A:LEU:H | 1:36:A:LEU:HB3 | 5 | 0.11 |
| (2,165) | 1:42:A:LEU:HA | 1:42:A:LEU:HB3 | 5 | 0.11 |
| (2,165) | 1:42:A:LEU:HA | 1:42:A:LEU:HB3 | 8 | 0.11 |
| (2,153) | 1:51:A:GLN:HE21 | 1:60:A:ILE:HA | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,153) | 1:51:A:GLN:HE21 | 1:60:A:ILE:HA | 15 | 0.11 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 11 | 0.11 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 18 | 0.11 |
| (2,129) | 1:79:A:LEU:HG | 1:76:A:ASP:HB2 | 13 | 0.11 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 1 | 0.11 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 7 | 0.11 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 12 | 0.11 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 16 | 0.11 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 17 | 0.11 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 19 | 0.11 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 1 | 0.11 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 2 | 0.11 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 7 | 0.11 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 16 | 0.11 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 20 | 0.11 |
| (2,80) | 1:51:A:GLN:HE21 | 1:63:A:GLU:HB2 | 11 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 2 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 3 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 4 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 6 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 13 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 14 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 15 | 0.11 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 17 | 0.11 |
| (2,55) | 1:45:A:VAL:HB | 1:83:A:ASN:HA | 11 | 0.11 |
| (2,44) | 1:51:A:GLN:HB2 | 1:50:A:THR:HA | 11 | 0.11 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 5 | 0.11 |
| (1,6) | 1:36:A:LEU:H | 1:36:A:LEU:HA | 8 | 0.11 |
| (1,5) | 1:45:A:VAL:HG22 | 1:45:A:VAL:HB | 5 | 0.11 |
| (2,1278) | 1:38:A:THR:HA | 1:41:A:VAL:H | 4 | 0.1 |
| (2,1189) | 1:54:A:LEU:H | 1:54:A:LEU:HA | 8 | 0.1 |
| (2,1189) | 1:54:A:LEU:H | 1:54:A:LEU:HA | 10 | 0.1 |
| (2,1142) | 1:24:A:LYS:H | 1:24:A:LYS:HG3 | 16 | 0.1 |
| (2,1128) | 1:23:A:LYS:HB3 | 1:22:A:ASN:H | 4 | 0.1 |
| (2,1077) | 1:28:A:SER:HB2 | 1:29:A:THR:H | 10 | 0.1 |
| (2,1068) | 1:47:A:ILE:HG23 | 1:21:A:THR:H | 11 | 0.1 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 14 | 0.1 |
| (2,1034) | 1:73:A:ASP:HA | 1:33:A:SER:H | 17 | 0.1 |
| (2,1024) | 1:85:A:THR:HG23 | 1:85:A:THR:H | 9 | 0.1 |
| (2,1024) | 1:85:A:THR:HG22 | 1:85:A:THR:H | 20 | 0.1 |
| (2,960) | 1:7:A:LYS:HG3 | 1:8:A:THR:H | 7 | 0.1 |
| (2,927) | 1:46:A:ALA:H | 1:45:A:VAL:H | 4 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,923) | 1:21:A:THR:HG23 | 1:67:A:THR:HB | 10 | 0.1 |
| (2,913) | 1:61:A:GLU:H | 1:61:A:GLU:HG3 | 11 | 0.1 |
| (2,889) | 1:47:A:ILE:HD13 | 1:19:A:CYS:HA | 7 | 0.1 |
| (2,889) | 1:47:A:ILE:HD11 | 1:19:A:CYS:HA | 10 | 0.1 |
| (2,889) | 1:47:A:ILE:HD12 | 1:19:A:CYS:HA | 14 | 0.1 |
| (2,883) | 1:73:A:ASP:HA | 1:15:A:LYS:HD3 | 1 | 0.1 |
| (2,880) | 1:60:A:ILE:HA | 1:64:A:CYS:HB3 | 3 | 0.1 |
| (2,878) | 1:90:A:ILE:H | 1:89:A:LEU:HB3 | 17 | 0.1 |
| (2,872) | 1:21:A:THR:H | 1:20:A:ASP:HB2 | 2 | 0.1 |
| (2,797) | 1:25:A:VAL:H | 1:24:A:LYS:HB2 | 2 | 0.1 |
| (2,644) | 1:63:A:GLU:HA | 1:63:A:GLU:HG2 | 12 | 0.1 |
| (2,628) | 1:88:A:PRO:HD2 | 1:88:A:PRO:HB3 | 9 | 0.1 |
| (2,628) | 1:88:A:PRO:HD2 | 1:88:A:PRO:HB3 | 18 | 0.1 |
| (2,609) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HG2 | 5 | 0.1 |
| (2,609) | 1:86:A:PRO:HD3 | 1:86:A:PRO:HG2 | 9 | 0.1 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 1 | 0.1 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 2 | 0.1 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 5 | 0.1 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 11 | 0.1 |
| (2,594) | 1:16:A:LEU:H | 1:16:A:LEU:HG | 17 | 0.1 |
| (2,592) | 1:50:A:THR:H | 1:49:A:CYS:HB2 | 16 | 0.1 |
| (2,513) | 1:57:A:GLY:HA3 | 1:56:A:ILE:HG23 | 16 | 0.1 |
| (2,484) | 1:87:A:ILE:HG22 | 1:88:A:PRO:HD2 | 17 | 0.1 |
| (2,428) | 1:59:A:ALA:HB3 | 1:62:A:ASP:HB3 | 3 | 0.1 |
| (2,405) | 1:82:A:ILE:HG23 | 1:72:A:GLU:HG3 | 11 | 0.1 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 15 | 0.1 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 17 | 0.1 |
| (2,378) | 1:72:A:GLU:HB3 | 1:83:A:ASN:HB3 | 19 | 0.1 |
| (2,267) | 1:36:A:LEU:HD11 | 1:36:A:LEU:HA | 16 | 0.1 |
| (2,180) | 1:69:A:THR:HG23 | 1:86:A:PRO:HB2 | 14 | 0.1 |
| (2,174) | 1:83:A:ASN:H | 1:82:A:ILE:HG22 | 17 | 0.1 |
| (2,165) | 1:42:A:LEU:HA | 1:42:A:LEU:HB3 | 6 | 0.1 |
| (2,153) | 1:51:A:GLN:HE21 | 1:60:A:ILE:HA | 19 | 0.1 |
| (2,152) | 1:51:A:GLN:HE22 | 1:60:A:ILE:HA | 1 | 0.1 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 5 | 0.1 |
| (2,149) | 1:60:A:ILE:HG12 | 1:60:A:ILE:HA | 19 | 0.1 |
| (2,139) | 1:24:A:LYS:HA | 1:24:A:LYS:HD3 | 1 | 0.1 |
| (2,129) | 1:79:A:LEU:HG | 1:76:A:ASP:HB2 | 9 | 0.1 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 8 | 0.1 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 18 | 0.1 |
| (2,122) | 1:86:A:PRO:HB2 | 1:86:A:PRO:HA | 20 | 0.1 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 8 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 12 | 0.1 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 15 | 0.1 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 17 | 0.1 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 18 | 0.1 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 19 | 0.1 |
| (2,121) | 1:86:A:PRO:HD2 | 1:86:A:PRO:HA | 20 | 0.1 |
| (2,105) | 1:82:A:ILE:H | 1:71:A:CYS:HB2 | 13 | 0.1 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 2 | 0.1 |
| (2,94) | 1:87:A:ILE:H | 1:87:A:ILE:HB | 3 | 0.1 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 7 | 0.1 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 10 | 0.1 |
| (2,76) | 1:88:A:PRO:HD3 | 1:88:A:PRO:HB2 | 18 | 0.1 |
| (1,5) | 1:45:A:VAL:HG21 | 1:45:A:VAL:HB | 2 | 0.1 |
| (1,5) | 1:45:A:VAL:HG21 | 1:45:A:VAL:HB | 6 | 0.1 |
| (1,5) | 1:45:A:VAL:HG21 | 1:45:A:VAL:HB | 9 | 0.1 |
| (1,5) | 1:45:A:VAL:HG11 | 1:45:A:VAL:HB | 17 | 0.1 |
| (1,5) | 1:45:A:VAL:HG21 | 1:45:A:VAL:HB | 18 | 0.1 |

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

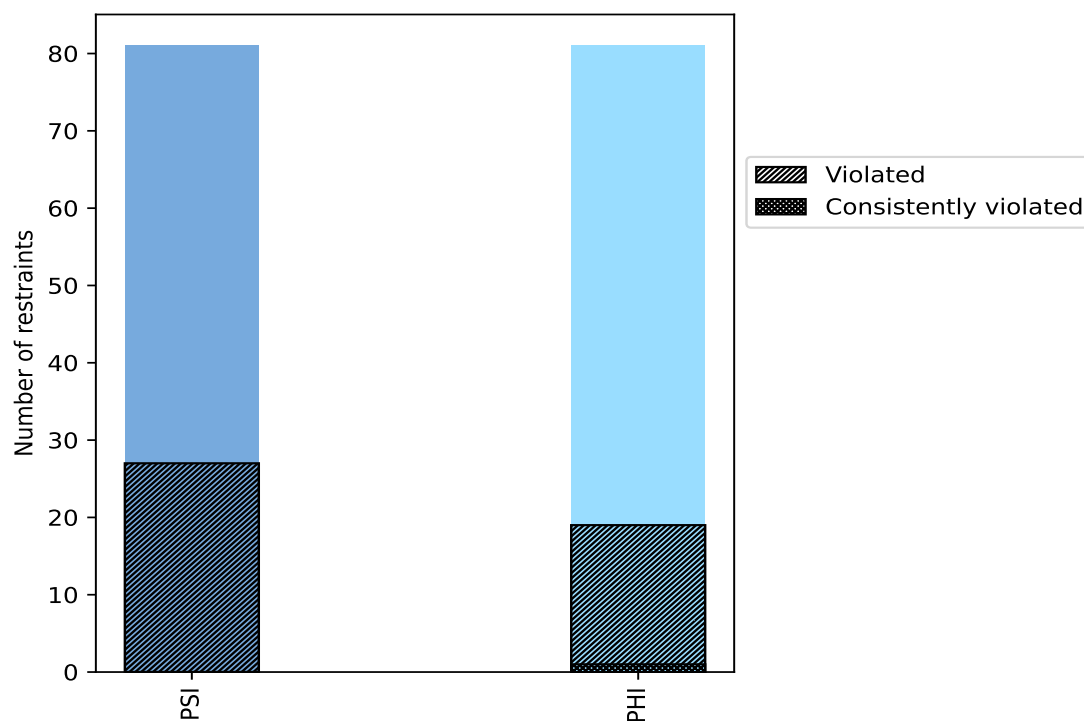
10.1 Summary of dihedral-angle violations [i](#)

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 |
| PSI | 81 | 50.0 | 27 | 33.3 | 16.7 | 0 | 0.0 | 0.0 |
| PHI | 81 | 50.0 | 19 | 23.5 | 11.7 | 1 | 1.2 | 0.6 |
| Total | 162 | 100.0 | 46 | 28.4 | 28.4 | 1 | 0.6 | 0.6 |

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](#)



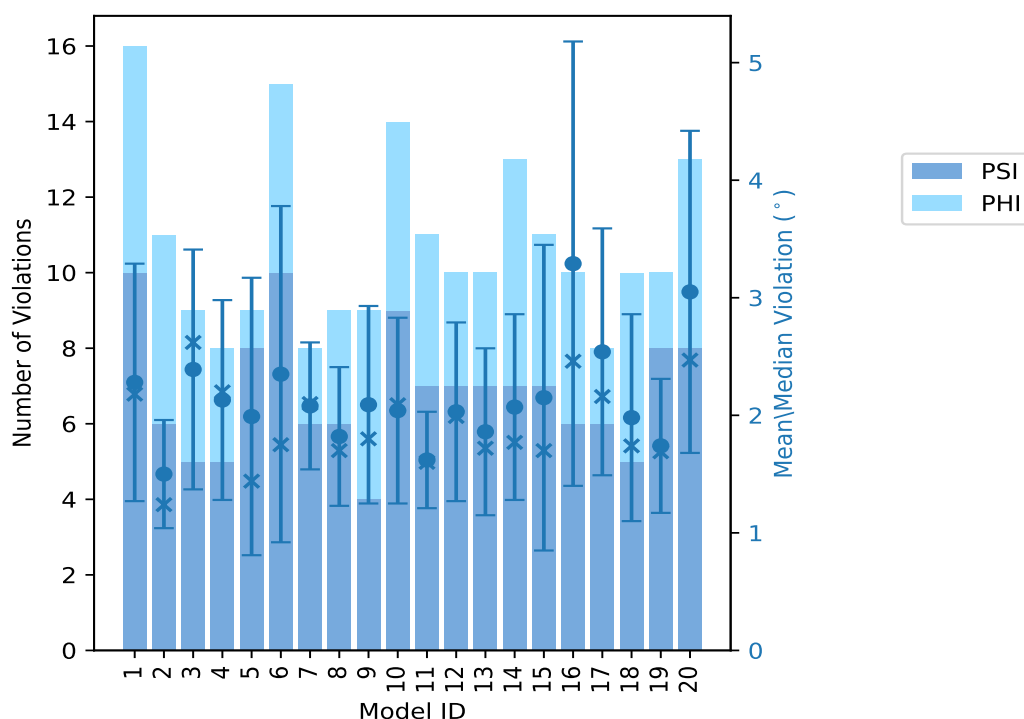
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 1 | 10 | 6 | 16 | 2.28 | 4.08 | 1.01 | 2.18 |
| 2 | 6 | 5 | 11 | 1.5 | 2.41 | 0.46 | 1.24 |
| 3 | 5 | 4 | 9 | 2.39 | 3.87 | 1.02 | 2.62 |
| 4 | 5 | 3 | 8 | 2.13 | 3.32 | 0.85 | 2.2 |
| 5 | 8 | 1 | 9 | 1.99 | 4.61 | 1.18 | 1.44 |
| 6 | 10 | 5 | 15 | 2.35 | 5.33 | 1.43 | 1.75 |
| 7 | 6 | 2 | 8 | 2.08 | 2.94 | 0.54 | 2.1 |
| 8 | 6 | 3 | 9 | 1.82 | 2.71 | 0.59 | 1.7 |
| 9 | 4 | 5 | 9 | 2.09 | 3.41 | 0.84 | 1.8 |
| 10 | 9 | 5 | 14 | 2.04 | 3.95 | 0.79 | 2.09 |
| 11 | 7 | 4 | 11 | 1.62 | 2.41 | 0.41 | 1.6 |
| 12 | 7 | 3 | 10 | 2.03 | 3.42 | 0.76 | 1.99 |
| 13 | 7 | 3 | 10 | 1.86 | 3.69 | 0.71 | 1.72 |
| 14 | 7 | 6 | 13 | 2.07 | 3.7 | 0.79 | 1.77 |
| 15 | 7 | 4 | 11 | 2.15 | 5.22 | 1.3 | 1.7 |
| 16 | 6 | 4 | 10 | 3.29 | 7.81 | 1.89 | 2.46 |
| 17 | 6 | 2 | 8 | 2.54 | 4.6 | 1.05 | 2.16 |
| 18 | 5 | 5 | 10 | 1.98 | 3.37 | 0.88 | 1.74 |
| 19 | 8 | 2 | 10 | 1.74 | 3.02 | 0.57 | 1.69 |
| 20 | 8 | 5 | 13 | 3.05 | 5.37 | 1.37 | 2.47 |

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



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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|------|
| PSI | PHI | Total | Count ¹ | % |
| 5 | 8 | 13 | 1 | 5.0 |
| 5 | 3 | 8 | 2 | 10.0 |
| 4 | 2 | 6 | 3 | 15.0 |
| 0 | 1 | 1 | 4 | 20.0 |
| 5 | 1 | 6 | 5 | 25.0 |
| 2 | 0 | 2 | 6 | 30.0 |
| 1 | 1 | 2 | 7 | 35.0 |
| 0 | 1 | 1 | 8 | 40.0 |
| 1 | 0 | 1 | 9 | 45.0 |
| 1 | 0 | 1 | 10 | 50.0 |
| 0 | 0 | 0 | 11 | 55.0 |

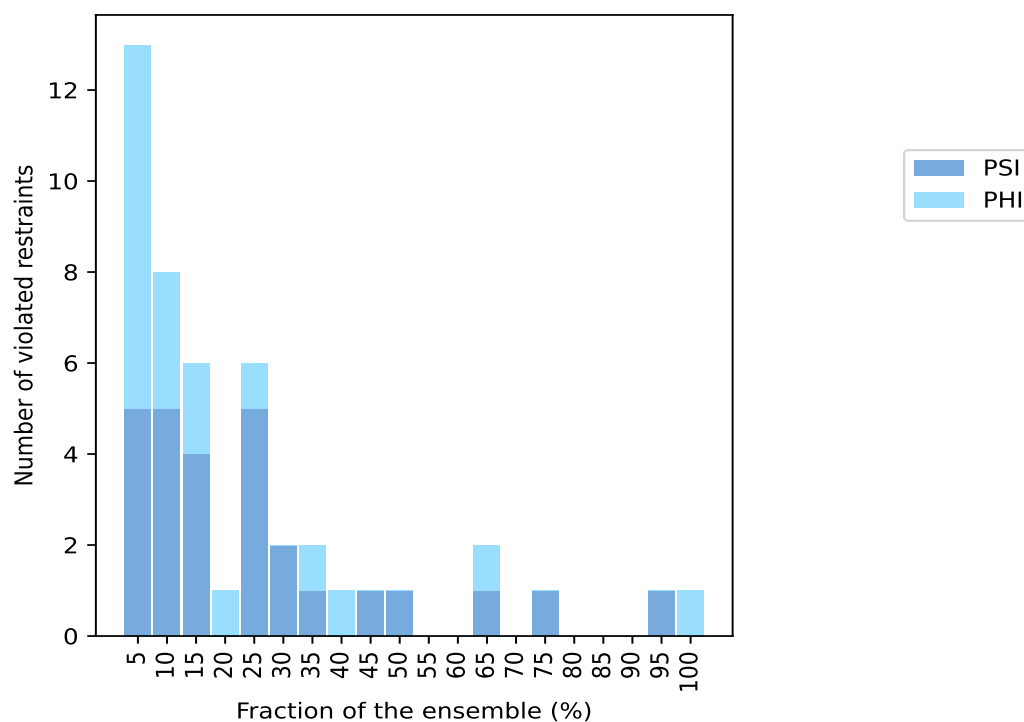
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 1 | 1 | 2 | 13 | 65.0 |
| 0 | 0 | 0 | 14 | 70.0 |
| 1 | 0 | 1 | 15 | 75.0 |
| 0 | 0 | 0 | 16 | 80.0 |
| 0 | 0 | 0 | 17 | 85.0 |
| 0 | 0 | 0 | 18 | 90.0 |
| 1 | 0 | 1 | 19 | 95.0 |
| 0 | 1 | 1 | 20 | 100.0 |

¹ Number of models with violations

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

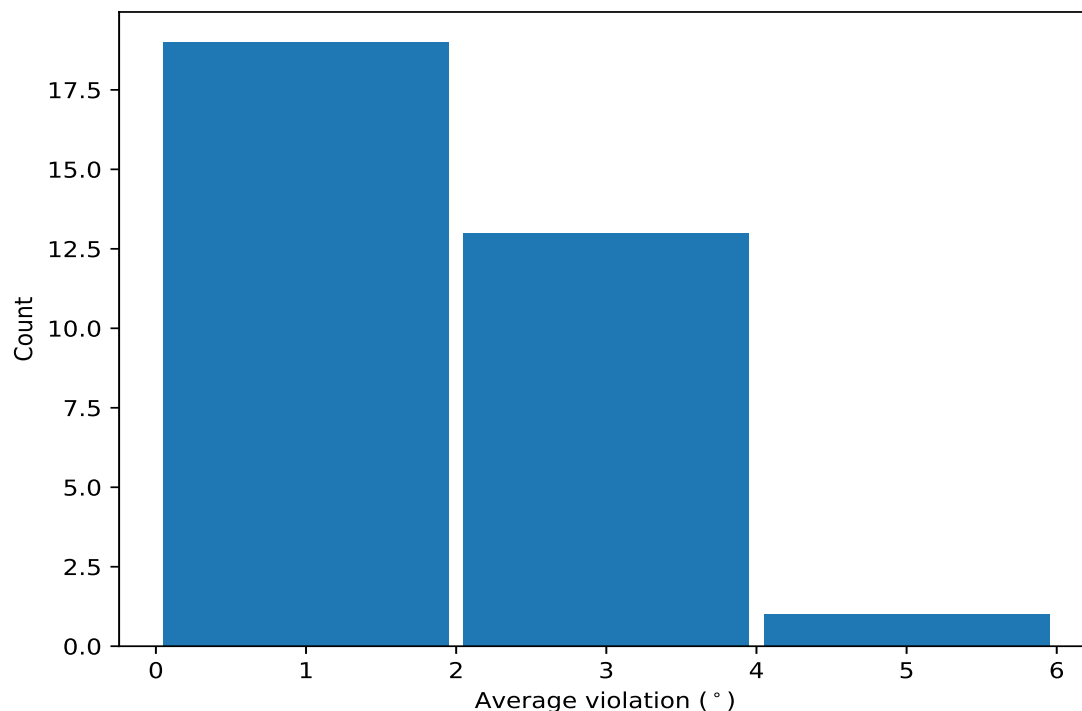


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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 |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 20 | 3.0 | 1.21 | 3.08 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 19 | 3.34 | 1.1 | 3.42 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 15 | 1.76 | 0.37 | 1.73 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 13 | 2.34 | 0.67 | 2.12 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 13 | 1.88 | 0.39 | 1.91 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 10 | 2.11 | 0.86 | 1.86 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 9 | 1.87 | 0.58 | 1.77 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 8 | 1.8 | 0.76 | 1.37 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 7 | 2.05 | 0.42 | 2.33 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 7 | 1.25 | 0.23 | 1.13 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 6 | 1.8 | 0.67 | 1.7 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 6 | 1.3 | 0.32 | 1.16 |
| (1,58) | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 1:37:A:HIS:N | 5 | 3.16 | 1.2 | 2.93 |
| (1,46) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:SER:N | 5 | 2.74 | 1.96 | 1.26 |
| (1,3) | 1:5:A:GLU:C | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 5 | 2.23 | 0.76 | 1.75 |
| (1,94) | 1:54:A:LEU:N | 1:54:A:LEU:CA | 1:54:A:LEU:C | 1:55:A:LEU:N | 5 | 2.11 | 0.3 | 2.14 |
| (1,60) | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1:38:A:THR:N | 5 | 1.56 | 0.44 | 1.39 |
| (1,72) | 1:43:A:ASP:N | 1:43:A:ASP:CA | 1:43:A:ASP:C | 1:44:A:GLN:N | 5 | 1.5 | 0.23 | 1.43 |
| (1,47) | 1:30:A:GLY:C | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 4 | 1.98 | 0.86 | 1.66 |
| (1,59) | 1:36:A:LEU:C | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 3 | 2.95 | 1.29 | 2.22 |

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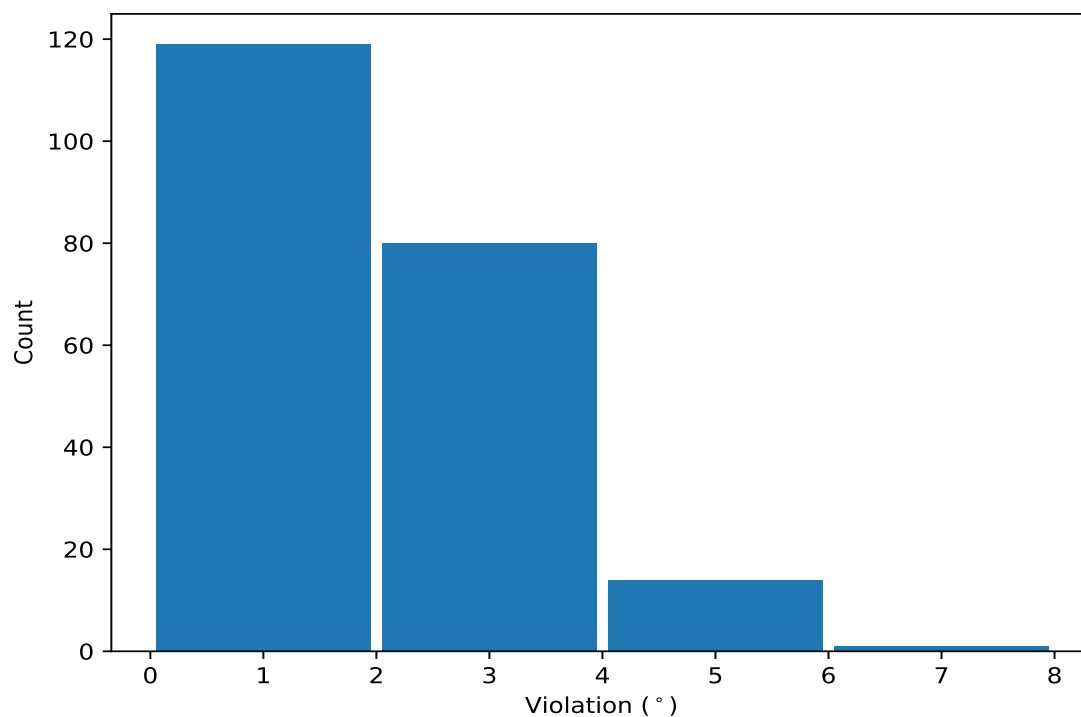
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,12) | 1:10:A:SER:N | 1:10:A:SER:CA | 1:10:A:SER:C | 1:11:A:CYS:N | 3 | 1.71 | 0.45 | 2.01 |
| (1,141) | 1:77:A:ASP:C | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 3 | 1.5 | 0.5 | 1.2 |
| (1,26) | 1:17:A:ALA:N | 1:17:A:ALA:CA | 1:17:A:ALA:C | 1:18:A:CYS:N | 3 | 1.4 | 0.06 | 1.36 |
| (1,48) | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 1:32:A:GLU:N | 3 | 1.26 | 0.21 | 1.13 |
| (1,112) | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 1:64:A:CYS:N | 3 | 1.15 | 0.01 | 1.16 |
| (1,45) | 1:26:A:GLN:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 2 | 4.46 | 3.34 | 4.46 |
| (1,44) | 1:26:A:GLN:N | 1:26:A:GLN:CA | 1:26:A:GLN:C | 1:27:A:LYS:N | 2 | 3.06 | 0.56 | 3.06 |
| (1,54) | 1:34:A:GLY:N | 1:34:A:GLY:CA | 1:34:A:GLY:C | 1:35:A:LEU:N | 2 | 2.89 | 1.19 | 2.89 |
| (1,56) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:LEU:N | 2 | 2.45 | 0.5 | 2.45 |
| (1,16) | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 1:13:A:THR:N | 2 | 1.74 | 0.14 | 1.74 |
| (1,51) | 1:32:A:GLU:C | 1:33:A:SER:N | 1:33:A:SER:CA | 1:33:A:SER:C | 2 | 1.69 | 0.52 | 1.69 |
| (1,66) | 1:40:A:ASP:N | 1:40:A:ASP:CA | 1:40:A:ASP:C | 1:41:A:VAL:N | 2 | 1.4 | 0.34 | 1.4 |
| (1,115) | 1:64:A:CYS:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 2 | 1.25 | 0.1 | 1.25 |

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 (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,45) | 1:26:A:GLN:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 16 | 7.81 |
| (1,46) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:SER:N | 16 | 5.47 |
| (1,58) | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 1:37:A:HIS:N | 20 | 5.37 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 6 | 5.33 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 15 | 5.22 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 20 | 5.04 |
| (1,46) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:SER:N | 6 | 4.79 |
| (1,59) | 1:36:A:LEU:C | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 20 | 4.76 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 6 | 4.68 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 5 | 4.61 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 17 | 4.6 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 20 | 4.54 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 15 | 4.44 |
| (1,54) | 1:34:A:GLY:N | 1:34:A:GLY:CA | 1:34:A:GLY:C | 1:35:A:LEU:N | 1 | 4.08 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 16 | 4.06 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 10 | 3.95 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 17 | 3.88 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 3 | 3.87 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 14 | 3.7 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 13 | 3.69 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 1 | 3.67 |
| (1,44) | 1:26:A:GLN:N | 1:26:A:GLN:CA | 1:26:A:GLN:C | 1:27:A:LYS:N | 6 | 3.63 |
| (1,57) | 1:35:A:LEU:C | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 20 | 3.59 |
| (1,3) | 1:5:A:GLU:C | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 3 | 3.54 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 5 | 3.45 |
| (1,47) | 1:30:A:GLY:C | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 1 | 3.43 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 12 | 3.42 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 9 | 3.41 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 18 | 3.37 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 1 | 3.36 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 4 | 3.32 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 3 | 3.32 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 18 | 3.27 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 1 | 3.22 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 4 | 3.18 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 9 | 3.17 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 12 | 3.13 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 9 | 3.13 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 16 | 3.09 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 14 | 3.08 |
| (1,58) | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 1:37:A:HIS:N | 18 | 3.03 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 19 | 3.02 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 14 | 2.95 |
| (1,56) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:LEU:N | 20 | 2.95 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 7 | 2.94 |
| (1,58) | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 1:37:A:HIS:N | 1 | 2.93 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 3 | 2.87 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,58) | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 1:37:A:HIS:N | 10 | 2.8 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 10 | 2.8 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 8 | 2.71 |
| (1,94) | 1:54:A:LEU:N | 1:54:A:LEU:CA | 1:54:A:LEU:C | 1:55:A:LEU:N | 4 | 2.63 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 14 | 2.63 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 3 | 2.62 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 7 | 2.62 |
| (1,3) | 1:5:A:GLU:C | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 4 | 2.61 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 12 | 2.55 |
| (1,6) | 1:7:A:LYS:N | 1:7:A:LYS:CA | 1:7:A:LYS:C | 1:8:A:THR:N | 8 | 2.52 |
| (1,44) | 1:26:A:GLN:N | 1:26:A:GLN:CA | 1:26:A:GLN:C | 1:27:A:LYS:N | 16 | 2.5 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 20 | 2.47 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 16 | 2.43 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 16 | 2.43 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 10 | 2.42 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 2 | 2.41 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 11 | 2.41 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 7 | 2.37 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 13 | 2.36 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 1 | 2.34 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 8 | 2.33 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 2 | 2.32 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 10 | 2.31 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 14 | 2.31 |
| (1,60) | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1:38:A:THR:N | 11 | 2.3 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 14 | 2.3 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 19 | 2.26 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 5 | 2.25 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 17 | 2.24 |
| (1,59) | 1:36:A:LEU:C | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 10 | 2.22 |
| (1,51) | 1:32:A:GLU:C | 1:33:A:SER:N | 1:33:A:SER:CA | 1:33:A:SER:C | 1 | 2.21 |
| (1,141) | 1:77:A:ASP:C | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 17 | 2.2 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 10 | 2.2 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 8 | 2.18 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 7 | 2.16 |
| (1,94) | 1:54:A:LEU:N | 1:54:A:LEU:CA | 1:54:A:LEU:C | 1:55:A:LEU:N | 1 | 2.15 |
| (1,94) | 1:54:A:LEU:N | 1:54:A:LEU:CA | 1:54:A:LEU:C | 1:55:A:LEU:N | 16 | 2.14 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 6 | 2.14 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 17 | 2.12 |
| (1,96) | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 1:56:A:ILE:N | 17 | 2.12 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 12 | 2.12 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 12 | 2.07 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 13 | 2.06 |
| (1,12) | 1:10:A:SER:N | 1:10:A:SER:CA | 1:10:A:SER:C | 1:11:A:CYS:N | 7 | 2.05 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 19 | 2.04 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 17 | 2.01 |
| (1,12) | 1:10:A:SER:N | 1:10:A:SER:CA | 1:10:A:SER:C | 1:11:A:CYS:N | 18 | 2.01 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 20 | 2.0 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 10 | 1.98 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 18 | 1.97 |
| (1,56) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:LEU:N | 6 | 1.95 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 20 | 1.93 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 6 | 1.92 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 12 | 1.91 |
| (1,94) | 1:54:A:LEU:N | 1:54:A:LEU:CA | 1:54:A:LEU:C | 1:55:A:LEU:N | 10 | 1.91 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 11 | 1.89 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 13 | 1.89 |
| (1,16) | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 1:13:A:THR:N | 15 | 1.89 |
| (1,59) | 1:36:A:LEU:C | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1 | 1.87 |
| (1,72) | 1:43:A:ASP:N | 1:43:A:ASP:CA | 1:43:A:ASP:C | 1:44:A:GLN:N | 9 | 1.81 |
| (1,60) | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1:38:A:THR:N | 15 | 1.81 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 9 | 1.8 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 4 | 1.79 |
| (1,47) | 1:30:A:GLY:C | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 20 | 1.78 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 15 | 1.78 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 2 | 1.77 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 14 | 1.77 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 6 | 1.75 |
| (1,3) | 1:5:A:GLU:C | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 14 | 1.75 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 20 | 1.75 |
| (1,72) | 1:43:A:ASP:N | 1:43:A:ASP:CA | 1:43:A:ASP:C | 1:44:A:GLN:N | 20 | 1.73 |
| (1,66) | 1:40:A:ASP:N | 1:40:A:ASP:CA | 1:40:A:ASP:C | 1:41:A:VAL:N | 20 | 1.73 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 5 | 1.73 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 19 | 1.73 |
| (1,94) | 1:54:A:LEU:N | 1:54:A:LEU:CA | 1:54:A:LEU:C | 1:55:A:LEU:N | 13 | 1.72 |
| (1,3) | 1:5:A:GLU:C | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 7 | 1.72 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 13 | 1.72 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 6 | 1.71 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 8 | 1.7 |
| (1,54) | 1:34:A:GLY:N | 1:34:A:GLY:CA | 1:34:A:GLY:C | 1:35:A:LEU:N | 15 | 1.7 |
| (1,58) | 1:36:A:LEU:N | 1:36:A:LEU:CA | 1:36:A:LEU:C | 1:37:A:HIS:N | 19 | 1.69 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 19 | 1.69 |
| (1,52) | 1:33:A:SER:N | 1:33:A:SER:CA | 1:33:A:SER:C | 1:34:A:GLY:N | 6 | 1.63 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 9 | 1.63 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 11 | 1.62 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 19 | 1.62 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 11 | 1.61 |
| (1,16) | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 1:13:A:THR:N | 11 | 1.6 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 16 | 1.6 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 2 | 1.58 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 2 | 1.55 |
| (1,69) | 1:41:A:VAL:C | 1:42:A:LEU:N | 1:42:A:LEU:CA | 1:42:A:LEU:C | 15 | 1.55 |
| (1,48) | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 1:32:A:GLU:N | 10 | 1.55 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 7 | 1.54 |
| (1,47) | 1:30:A:GLY:C | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 15 | 1.53 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 3 | 1.52 |
| (1,3) | 1:5:A:GLU:C | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 18 | 1.52 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 3 | 1.5 |
| (1,26) | 1:17:A:ALA:N | 1:17:A:ALA:CA | 1:17:A:ALA:C | 1:18:A:CYS:N | 1 | 1.49 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 11 | 1.49 |
| (1,55) | 1:34:A:GLY:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 9 | 1.48 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 5 | 1.44 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 15 | 1.43 |
| (1,72) | 1:43:A:ASP:N | 1:43:A:ASP:CA | 1:43:A:ASP:C | 1:44:A:GLN:N | 13 | 1.43 |
| (1,103) | 1:58:A:ILE:C | 1:59:A:ALA:N | 1:59:A:ALA:CA | 1:59:A:ALA:C | 9 | 1.4 |
| (1,60) | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1:38:A:THR:N | 8 | 1.39 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 14 | 1.38 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 13 | 1.37 |
| (1,26) | 1:17:A:ALA:N | 1:17:A:ALA:CA | 1:17:A:ALA:C | 1:18:A:CYS:N | 13 | 1.36 |
| (1,115) | 1:64:A:CYS:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 16 | 1.35 |
| (1,72) | 1:43:A:ASP:N | 1:43:A:ASP:CA | 1:43:A:ASP:C | 1:44:A:GLN:N | 1 | 1.35 |
| (1,28) | 1:18:A:CYS:N | 1:18:A:CYS:CA | 1:18:A:CYS:C | 1:19:A:CYS:N | 14 | 1.35 |
| (1,26) | 1:17:A:ALA:N | 1:17:A:ALA:CA | 1:17:A:ALA:C | 1:18:A:CYS:N | 12 | 1.35 |
| (1,111) | 1:62:A:ASP:C | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 14 | 1.34 |
| (1,109) | 1:61:A:GLU:C | 1:62:A:ASP:N | 1:62:A:ASP:CA | 1:62:A:ASP:C | 12 | 1.34 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 11 | 1.31 |
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 12 | 1.31 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 4 | 1.29 |
| (1,91) | 1:52:A:ILE:C | 1:53:A:PRO:N | 1:53:A:PRO:CA | 1:53:A:PRO:C | 3 | 1.28 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 19 | 1.27 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 8 | 1.27 |
| (1,95) | 1:54:A:LEU:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 14 | 1.26 |
| (1,46) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:SER:N | 11 | 1.26 |
| (1,60) | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1:38:A:THR:N | 6 | 1.25 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 2 | 1.24 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 7 | 1.21 |
| (1,141) | 1:77:A:ASP:C | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 10 | 1.2 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 18 | 1.2 |
| (1,140) | 1:77:A:ASP:N | 1:77:A:ASP:CA | 1:77:A:ASP:C | 1:78:A:GLY:N | 4 | 1.19 |
| (1,72) | 1:43:A:ASP:N | 1:43:A:ASP:CA | 1:43:A:ASP:C | 1:44:A:GLN:N | 15 | 1.19 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 2 | 1.19 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 2 | 1.18 |
| (1,51) | 1:32:A:GLU:C | 1:33:A:SER:N | 1:33:A:SER:CA | 1:33:A:SER:C | 6 | 1.18 |
| (1,47) | 1:30:A:GLY:C | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 8 | 1.18 |
| (1,142) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1:79:A:LEU:N | 18 | 1.16 |
| (1,115) | 1:64:A:CYS:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 1 | 1.16 |
| (1,112) | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 1:64:A:CYS:N | 5 | 1.16 |
| (1,112) | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 1:64:A:CYS:N | 6 | 1.16 |
| (1,46) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:SER:N | 2 | 1.16 |
| (1,14) | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1:12:A:ASN:N | 11 | 1.16 |
| (1,112) | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 1:64:A:CYS:N | 14 | 1.14 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 5 | 1.14 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 18 | 1.13 |
| (1,48) | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 1:32:A:GLU:N | 17 | 1.13 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 11 | 1.13 |
| (1,45) | 1:26:A:GLN:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 6 | 1.12 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 5 | 1.12 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 1 | 1.11 |
| (1,15) | 1:11:A:CYS:C | 1:12:A:ASN:N | 1:12:A:ASN:CA | 1:12:A:ASN:C | 2 | 1.11 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 10 | 1.1 |
| (1,22) | 1:15:A:LYS:N | 1:15:A:LYS:CA | 1:15:A:LYS:C | 1:16:A:LEU:N | 15 | 1.1 |
| (1,141) | 1:77:A:ASP:C | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C | 18 | 1.09 |
| (1,48) | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C | 1:32:A:GLU:N | 12 | 1.09 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,4) | 1:6:A:SER:N | 1:6:A:SER:CA | 1:6:A:SER:C | 1:7:A:LYS:N | 8 | 1.08 |
| (1,60) | 1:37:A:HIS:N | 1:37:A:HIS:CA | 1:37:A:HIS:C | 1:38:A:THR:N | 10 | 1.07 |
| (1,42) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLN:N | 4 | 1.07 |
| (1,12) | 1:10:A:SER:N | 1:10:A:SER:CA | 1:10:A:SER:C | 1:11:A:CYS:N | 10 | 1.07 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 6 | 1.06 |
| (1,66) | 1:40:A:ASP:N | 1:40:A:ASP:CA | 1:40:A:ASP:C | 1:41:A:VAL:N | 1 | 1.06 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 1 | 1.05 |
| (1,2) | 1:5:A:GLU:N | 1:5:A:GLU:CA | 1:5:A:GLU:C | 1:6:A:SER:N | 5 | 1.05 |
| (1,13) | 1:10:A:SER:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 2 | 1.03 |
| (1,10) | 1:9:A:GLY:N | 1:9:A:GLY:CA | 1:9:A:GLY:C | 1:10:A:SER:N | 19 | 1.03 |
| (1,46) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:SER:N | 3 | 1.02 |
| (1,18) | 1:13:A:THR:N | 1:13:A:THR:CA | 1:13:A:THR:C | 1:14:A:GLY:N | 19 | 1.02 |
| (1,85) | 1:49:A:CYS:C | 1:50:A:THR:N | 1:50:A:THR:CA | 1:50:A:THR:C | 9 | 1.01 |
| (1,87) | 1:50:A:THR:C | 1:51:A:GLN:N | 1:51:A:GLN:CA | 1:51:A:GLN:C | 13 | 1.0 |