



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 03:33 PM EST

PDB ID : 6UCJ
BMRB ID : 50007
Title : proIAPP in DPC Micelles - Two-Conformer Ensemble Refinement, Open Conformer
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Deposited on : 2019-09-16

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

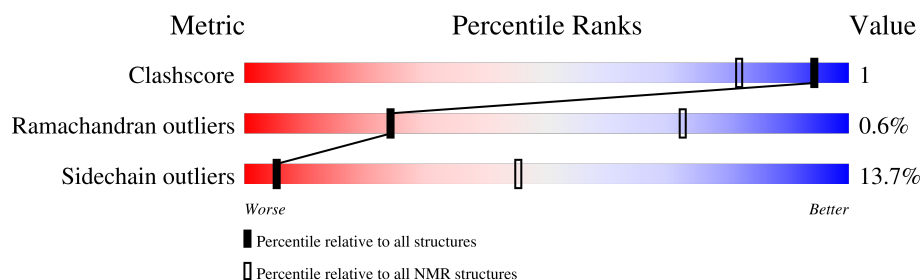
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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 | 72 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 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:3-A:15 (13) | 1.47 | 7 |
| 2 | A:21-A:66 (46) | 1.52 | 20 |

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

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

The models can be grouped into 4 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1044 atoms, of which 525 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Islet amyloid polypeptide.

| Mol | Chain | Residues | Atoms | | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|--|-------|
| 1 | A | 67 | Total | C | H | N | O | S | | 0 |
| | | | 1044 | 321 | 525 | 97 | 99 | 2 | | |

There are 5 discrepancies between the modelled and reference sequences:

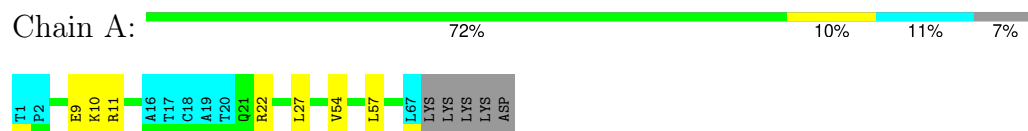
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 68 | LYS | - | expression tag | UNP P10997 |
| A | 69 | LYS | - | expression tag | UNP P10997 |
| A | 70 | LYS | - | expression tag | UNP P10997 |
| A | 71 | LYS | - | expression tag | UNP P10997 |
| A | 72 | ASP | - | expression tag | UNP P10997 |

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: Islet amyloid polypeptide

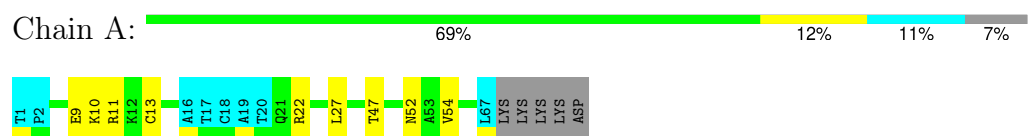


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

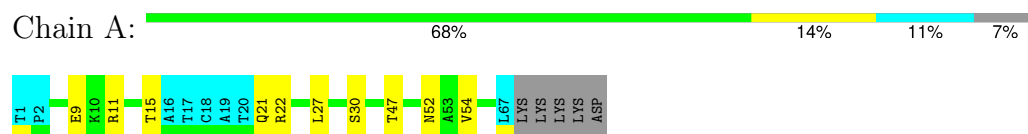
4.2.1 Score per residue for model 1

- Molecule 1: Islet amyloid polypeptide



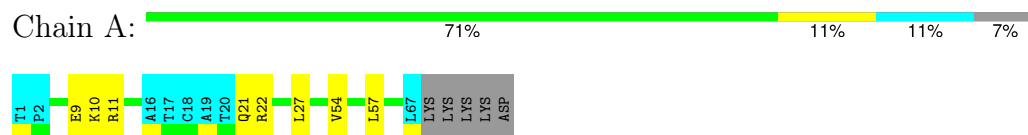
4.2.2 Score per residue for model 2

- Molecule 1: Islet amyloid polypeptide



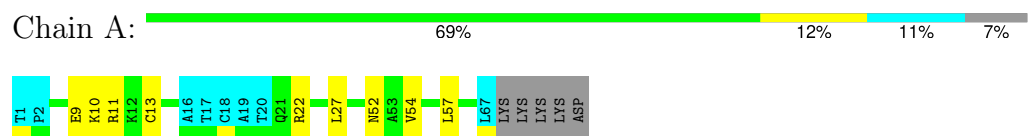
4.2.3 Score per residue for model 3

- Molecule 1: Islet amyloid polypeptide



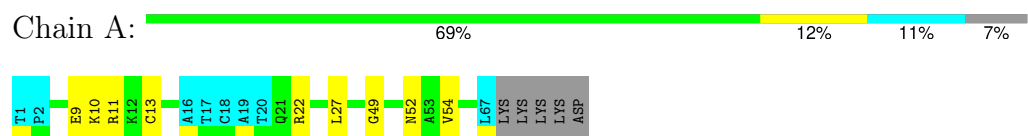
4.2.4 Score per residue for model 4

- Molecule 1: Islet amyloid polypeptide



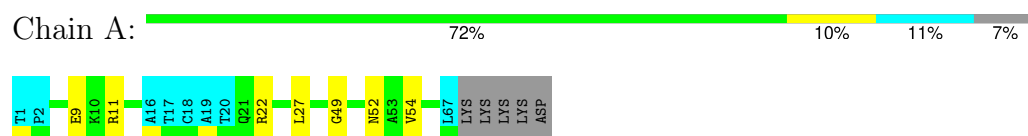
4.2.5 Score per residue for model 5

- Molecule 1: Islet amyloid polypeptide



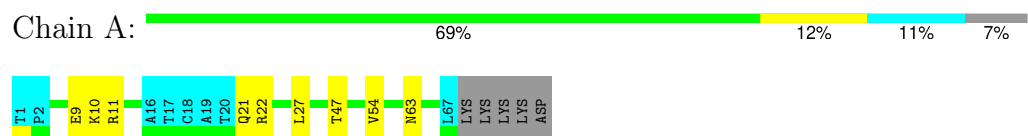
4.2.6 Score per residue for model 6

- Molecule 1: Islet amyloid polypeptide



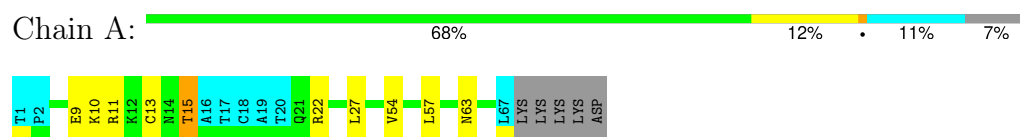
4.2.7 Score per residue for model 7

- Molecule 1: Islet amyloid polypeptide



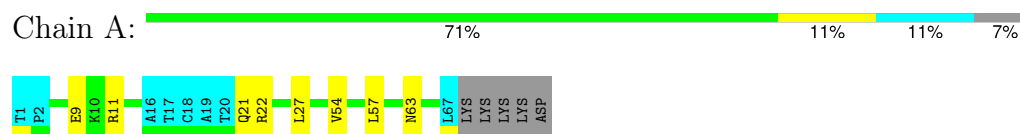
4.2.8 Score per residue for model 8

- Molecule 1: Islet amyloid polypeptide



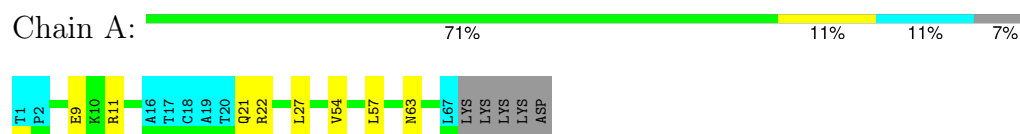
4.2.9 Score per residue for model 9

- Molecule 1: Islet amyloid polypeptide



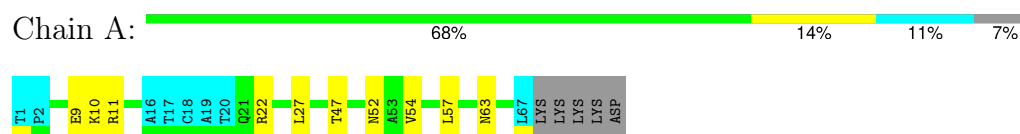
4.2.10 Score per residue for model 10

- Molecule 1: Islet amyloid polypeptide



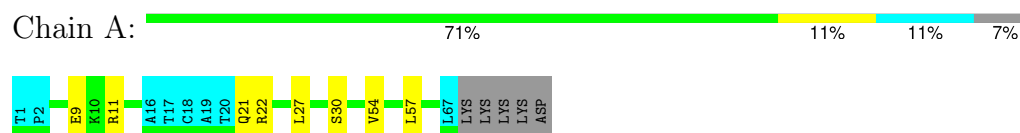
4.2.11 Score per residue for model 11

- Molecule 1: Islet amyloid polypeptide



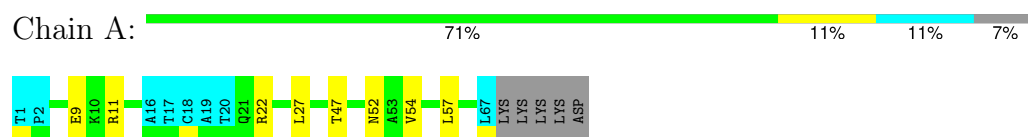
4.2.12 Score per residue for model 12

- Molecule 1: Islet amyloid polypeptide



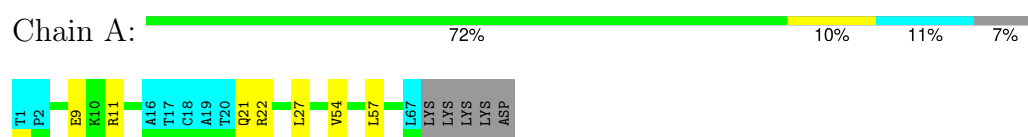
4.2.13 Score per residue for model 13

- Molecule 1: Islet amyloid polypeptide



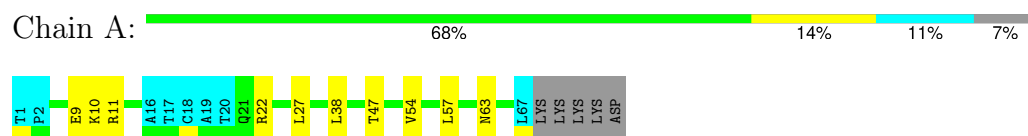
4.2.14 Score per residue for model 14

- Molecule 1: Islet amyloid polypeptide



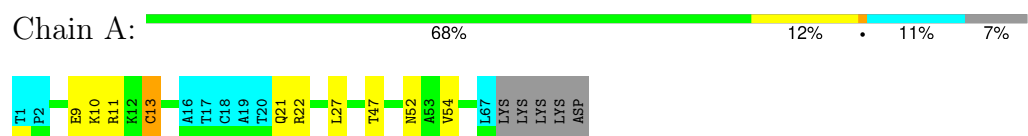
4.2.15 Score per residue for model 15

- Molecule 1: Islet amyloid polypeptide



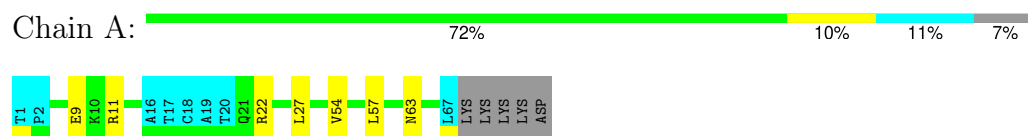
4.2.16 Score per residue for model 16

- Molecule 1: Islet amyloid polypeptide



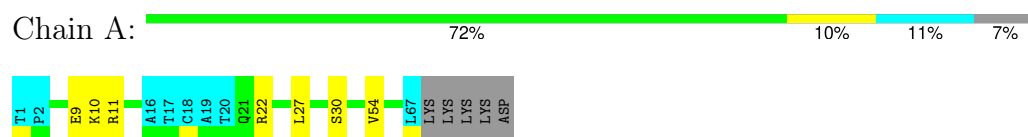
4.2.17 Score per residue for model 17

- Molecule 1: Islet amyloid polypeptide



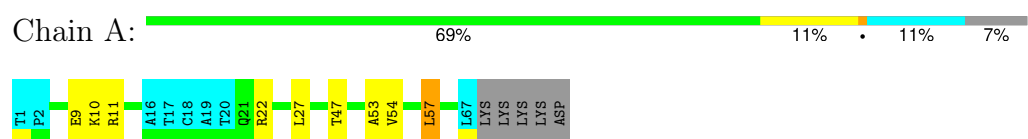
4.2.18 Score per residue for model 18

- Molecule 1: Islet amyloid polypeptide



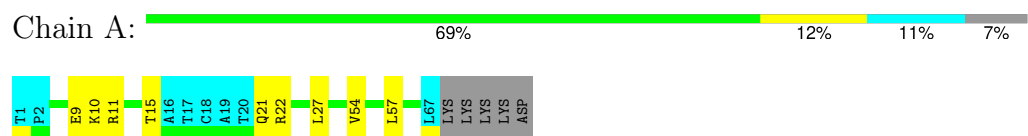
4.2.19 Score per residue for model 19

- Molecule 1: Islet amyloid polypeptide



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Islet amyloid polypeptide



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, simulated annealing*.

Of the 800 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 |
|---------------|-----------------------|---------|
| X-PLOR NIH | refinement | 2.48 |
| X-PLOR NIH | structure calculation | 2.48 |

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 | 822 |
| Number of shifts mapped to atoms | 757 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 65 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 83% |

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 | 467 | 470 | 468 | 1±0 |
| All | All | 9340 | 9400 | 9360 | 21 |

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 1.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:27:LEU:HD13 | 1:A:27:LEU:C | 0.44 | 2.33 | 20 | 19 |
| 1:A:13:CYS:SG | 1:A:15:THR:HG22 | 0.43 | 2.53 | 8 | 1 |
| 1:A:53:ALA:O | 1:A:57:LEU:HD13 | 0.40 | 2.17 | 19 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1 | A | 59/72 (82%) | 54±1 (92±2%) | 4±1 (7±2%) | 0±0 (1±1%) | 24 | 72 |
| All | All | 1180/1440 (82%) | 1087 (92%) | 86 (7%) | 7 (1%) | 24 | 72 |

All 3 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 | 15 | THR | 3 |
| 1 | A | 13 | CYS | 2 |
| 1 | A | 49 | GLY | 2 |

6.3.2 Protein sidechains ⓘ

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 | 53/64 (83%) | 46±1 (86±2%) | 7±1 (14±2%) | 5 | 45 |
| All | All | 1060/1280 (83%) | 915 (86%) | 145 (14%) | 5 | 45 |

All 14 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 | 9 | GLU | 20 |
| 1 | A | 11 | ARG | 20 |
| 1 | A | 22 | ARG | 20 |
| 1 | A | 54 | VAL | 20 |
| 1 | A | 57 | LEU | 13 |
| 1 | A | 10 | LYS | 12 |
| 1 | A | 21 | GLN | 9 |
| 1 | A | 47 | THR | 8 |
| 1 | A | 52 | ASN | 8 |
| 1 | A | 63 | ASN | 7 |
| 1 | A | 13 | CYS | 3 |
| 1 | A | 30 | SER | 3 |
| 1 | A | 27 | LEU | 1 |
| 1 | A | 38 | LEU | 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 83% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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 | 822 |
| Number of shifts mapped to atoms | 757 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 65 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

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

- No matching atom found in the structure. All 65 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 68 | LYS | C | 176.222 | 0.3 | 1 |
| 1 | A | 68 | LYS | CA | 56.09 | 0.3 | 1 |
| 1 | A | 68 | LYS | CB | 33.115 | 0.3 | 1 |
| 1 | A | 68 | LYS | CG | 24.567 | 0.3 | 1 |
| 1 | A | 68 | LYS | CD | 29.316 | 0.3 | 1 |
| 1 | A | 68 | LYS | CE | 42.009 | 0.3 | 1 |
| 1 | A | 68 | LYS | H | 8.197 | 0.020 | 1 |
| 1 | A | 68 | LYS | HA | 4.281 | 0.020 | 1 |
| 1 | A | 68 | LYS | HB2 | 1.79 | 0.020 | 2 |
| 1 | A | 68 | LYS | HB3 | 1.716 | 0.020 | 2 |
| 1 | A | 68 | LYS | HG2 | 1.424 | 0.020 | 1 |
| 1 | A | 68 | LYS | HG3 | 1.424 | 0.020 | 1 |
| 1 | A | 68 | LYS | HD2 | 1.576 | 0.020 | 1 |
| 1 | A | 68 | LYS | HD3 | 1.576 | 0.020 | 1 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 68 | LYS | N | 121.03 | 0.3 | 1 |
| 1 | A | 69 | LYS | C | 176.258 | 0.3 | 1 |
| 1 | A | 69 | LYS | CA | 56.192 | 0.3 | 1 |
| 1 | A | 69 | LYS | CB | 33.115 | 0.3 | 1 |
| 1 | A | 69 | LYS | CG | 24.48 | 0.3 | 1 |
| 1 | A | 69 | LYS | CD | 29.143 | 0.3 | 1 |
| 1 | A | 69 | LYS | CE | 42.009 | 0.3 | 1 |
| 1 | A | 69 | LYS | H | 8.258 | 0.020 | 1 |
| 1 | A | 69 | LYS | HA | 4.274 | 0.020 | 1 |
| 1 | A | 69 | LYS | HB2 | 1.775 | 0.020 | 2 |
| 1 | A | 69 | LYS | HB3 | 1.705 | 0.020 | 2 |
| 1 | A | 69 | LYS | HG2 | 1.411 | 0.020 | 1 |
| 1 | A | 69 | LYS | HG3 | 1.411 | 0.020 | 1 |
| 1 | A | 69 | LYS | HD2 | 1.575 | 0.020 | 1 |
| 1 | A | 69 | LYS | HD3 | 1.575 | 0.020 | 1 |
| 1 | A | 69 | LYS | HE2 | 2.992 | 0.020 | 1 |
| 1 | A | 69 | LYS | HE3 | 2.992 | 0.020 | 1 |
| 1 | A | 69 | LYS | N | 122.852 | 0.3 | 1 |
| 1 | A | 70 | LYS | C | 176.114 | 0.3 | 1 |
| 1 | A | 70 | LYS | CA | 56.293 | 0.3 | 1 |
| 1 | A | 70 | LYS | CB | 33.115 | 0.3 | 1 |
| 1 | A | 70 | LYS | CG | 24.567 | 0.3 | 1 |
| 1 | A | 70 | LYS | CD | 29.316 | 0.3 | 1 |
| 1 | A | 70 | LYS | CE | 42.009 | 0.3 | 1 |
| 1 | A | 70 | LYS | H | 8.299 | 0.020 | 1 |
| 1 | A | 70 | LYS | HA | 4.259 | 0.020 | 1 |
| 1 | A | 70 | LYS | HB2 | 1.776 | 0.020 | 2 |
| 1 | A | 70 | LYS | HB3 | 1.726 | 0.020 | 2 |
| 1 | A | 70 | LYS | HG2 | 1.411 | 0.020 | 1 |
| 1 | A | 70 | LYS | HG3 | 1.411 | 0.020 | 1 |
| 1 | A | 70 | LYS | HD2 | 1.655 | 0.020 | 1 |
| 1 | A | 70 | LYS | HD3 | 1.655 | 0.020 | 1 |
| 1 | A | 70 | LYS | N | 123.24 | 0.3 | 1 |
| 1 | A | 71 | LYS | C | 175.241 | 0.3 | 1 |
| 1 | A | 71 | LYS | CA | 56.361 | 0.3 | 1 |
| 1 | A | 71 | LYS | CB | 33.029 | 0.3 | 1 |
| 1 | A | 71 | LYS | CG | 24.567 | 0.3 | 1 |
| 1 | A | 71 | LYS | CD | 29.057 | 0.3 | 1 |
| 1 | A | 71 | LYS | CE | 41.923 | 0.3 | 1 |
| 1 | A | 71 | LYS | H | 8.332 | 0.020 | 1 |
| 1 | A | 71 | LYS | HA | 4.269 | 0.020 | 1 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 71 | LYS | HB2 | 1.813 | 0.020 | 2 |
| 1 | A | 71 | LYS | HB3 | 1.726 | 0.020 | 2 |
| 1 | A | 71 | LYS | N | 123.64 | 0.3 | 1 |
| 1 | A | 72 | ASP | CA | 55.071 | 0.3 | 1 |
| 1 | A | 72 | ASP | CB | 41.956 | 0.3 | 1 |
| 1 | A | 72 | ASP | H | 7.965 | 0.020 | 1 |
| 1 | A | 72 | ASP | HA | 4.289 | 0.020 | 1 |
| 1 | A | 72 | ASP | HB2 | 2.595 | 0.020 | 1 |
| 1 | A | 72 | ASP | HB3 | 2.595 | 0.020 | 1 |
| 1 | A | 72 | ASP | N | 126.551 | 0.3 | 1 |

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 71 | -0.24 ± 0.17 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 68 | 0.24 ± 0.08 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 69 | -0.03 ± 0.09 | None needed (< 0.5 ppm) |
| ^{15}N | 67 | 0.56 ± 0.25 | Should be applied |

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 83%, i.e. 679 atoms were assigned a chemical shift out of a possible 817. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 291/294 (99%) | 118/119 (99%) | 117/118 (99%) | 56/57 (98%) |
| Sidechain | 377/469 (80%) | 254/302 (84%) | 123/141 (87%) | 0/26 (0%) |
| Aromatic | 11/54 (20%) | 11/26 (42%) | 0/24 (0%) | 0/4 (0%) |
| Overall | 679/817 (83%) | 383/447 (86%) | 240/283 (85%) | 56/87 (64%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 757 atoms were assigned a chemical shift out of a possible 906. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|----------|---------------|---------------|-----------------|-----------------|
| Backbone | 324/332 (98%) | 131/134 (98%) | 131/134 (98%) | 62/64 (97%) |

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| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Sidechain | 422/520 (81%) | 285/337 (85%) | 137/157 (87%) | 0/26 (0%) |
| Aromatic | 11/54 (20%) | 11/26 (42%) | 0/24 (0%) | 0/4 (0%) |
| Overall | 757/906 (84%) | 427/497 (86%) | 268/315 (85%) | 62/94 (66%) |

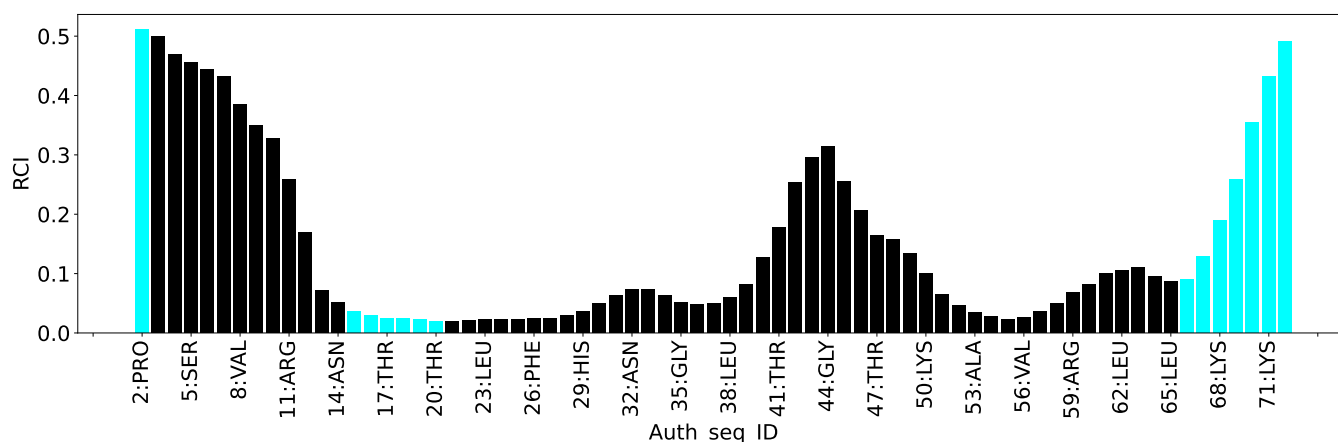
7.1.4 Statistically unusual chemical shifts [i](#)

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 | 477 |
| Intra-residue ($ i-j =0$) | 118 |
| Sequential ($ i-j =1$) | 208 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 127 |
| Long range ($ i-j \geq 5$) | 4 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 20 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 130 |
| Number of unmapped restraints | 1 |
| Number of restraints per residue | 8.4 |
| Number of long range restraints per residue ¹ | 0.1 |

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) | 18.4 | 0.2 |
| 0.2-0.5 (Medium) | 40.0 | 0.5 |
| >0.5 (Large) | 5.2 | 0.79 |

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) | 0.2 | 1.65 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

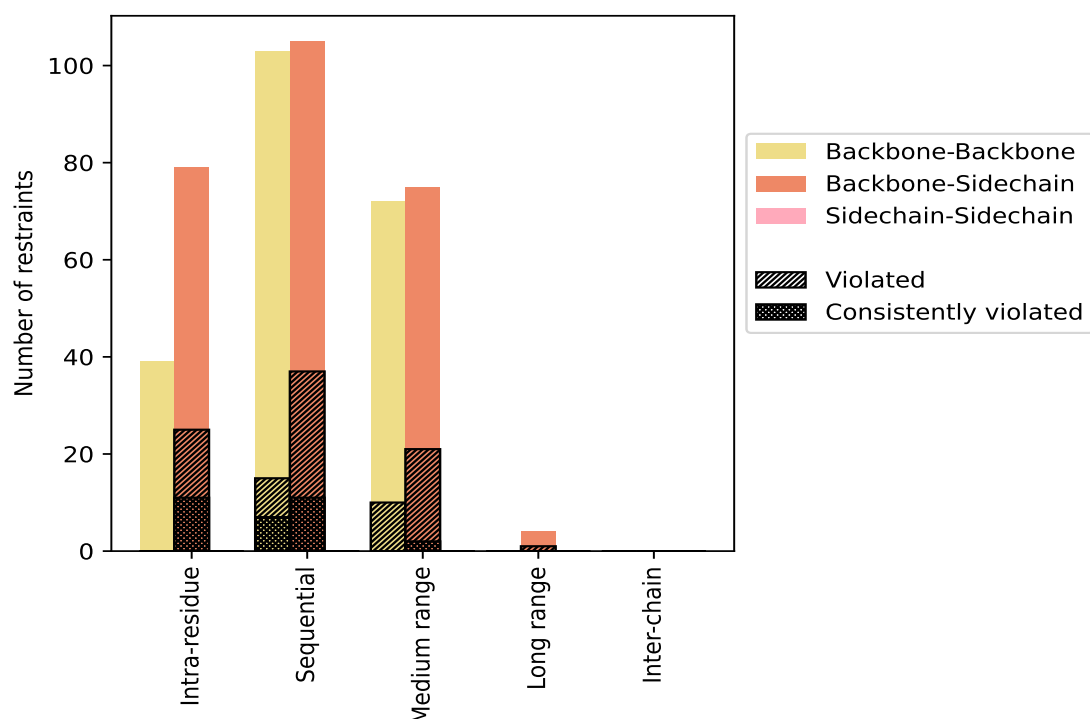
9.1 Summary of distance violations ⓘ

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|--|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|---------------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue (i-j =0) | 118 | 24.7 | 25 | 21.2 | 5.2 | 11 | 9.3 | 2.3 |
| Backbone-Backbone | 39 | 8.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 79 | 16.6 | 25 | 31.6 | 5.2 | 11 | 13.9 | 2.3 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential (i-j =1) | 208 | 43.6 | 52 | 25.0 | 10.9 | 18 | 8.7 | 3.8 |
| Backbone-Backbone | 103 | 21.6 | 15 | 14.6 | 3.1 | 7 | 6.8 | 1.5 |
| Backbone-Sidechain | 105 | 22.0 | 37 | 35.2 | 7.8 | 11 | 10.5 | 2.3 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Medium range (i-j >1 & i-j <5) | 127 | 26.6 | 16 | 12.6 | 3.4 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 72 | 15.1 | 10 | 13.9 | 2.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 55 | 11.5 | 6 | 10.9 | 1.3 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Long range (i-j ≥5) | 4 | 0.8 | 1 | 25.0 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 4 | 0.8 | 1 | 25.0 | 0.2 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| 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 | 20 | 4.2 | 15 | 75.0 | 3.1 | 2 | 10.0 | 0.4 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 477 | 100.0 | 109 | 22.9 | 22.9 | 31 | 6.5 | 6.5 |
| Backbone-Backbone | 214 | 44.9 | 25 | 11.7 | 5.2 | 7 | 3.3 | 1.5 |
| Backbone-Sidechain | 263 | 55.1 | 84 | 31.9 | 17.6 | 24 | 9.1 | 5.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |

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 | 18 | 31 | 17 | 0 | 0 | 66 | 0.3 | 0.62 | 0.12 | 0.28 |
| 2 | 18 | 38 | 15 | 0 | 0 | 71 | 0.28 | 0.68 | 0.12 | 0.25 |
| 3 | 16 | 31 | 12 | 0 | 0 | 59 | 0.3 | 0.7 | 0.13 | 0.29 |
| 4 | 18 | 30 | 19 | 0 | 0 | 67 | 0.29 | 0.6 | 0.14 | 0.26 |
| 5 | 16 | 32 | 16 | 0 | 0 | 64 | 0.29 | 0.58 | 0.13 | 0.24 |
| 6 | 16 | 33 | 14 | 0 | 0 | 63 | 0.3 | 0.57 | 0.12 | 0.26 |
| 7 | 17 | 33 | 13 | 0 | 0 | 63 | 0.28 | 0.73 | 0.15 | 0.24 |
| 8 | 16 | 37 | 14 | 0 | 0 | 67 | 0.29 | 0.7 | 0.15 | 0.23 |
| 9 | 15 | 32 | 16 | 0 | 0 | 63 | 0.29 | 0.77 | 0.14 | 0.29 |
| 10 | 17 | 35 | 15 | 0 | 0 | 67 | 0.29 | 0.79 | 0.14 | 0.26 |

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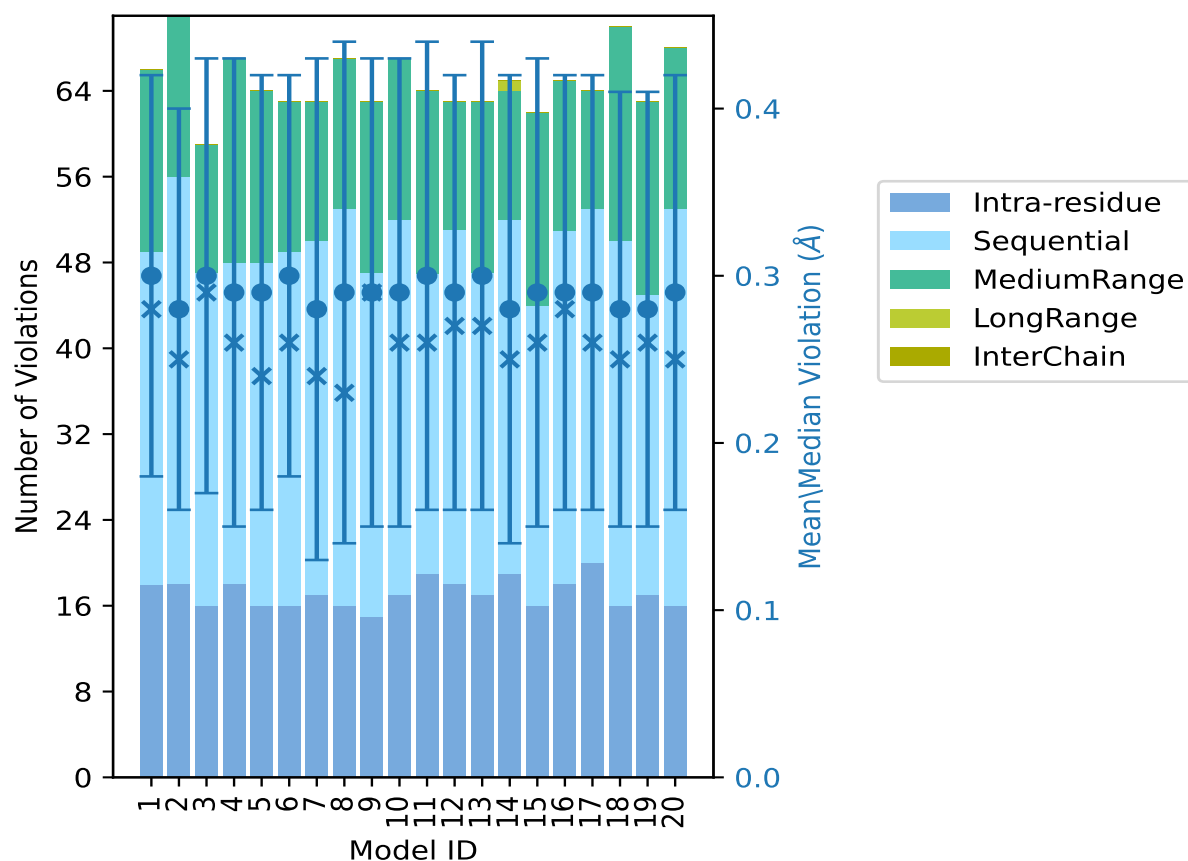
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 19 | 28 | 17 | 0 | 0 | 64 | 0.3 | 0.71 | 0.14 | 0.26 |
| 12 | 18 | 33 | 12 | 0 | 0 | 63 | 0.29 | 0.64 | 0.13 | 0.27 |
| 13 | 17 | 30 | 16 | 0 | 0 | 63 | 0.3 | 0.72 | 0.14 | 0.27 |
| 14 | 19 | 33 | 12 | 1 | 0 | 65 | 0.28 | 0.77 | 0.14 | 0.25 |
| 15 | 16 | 28 | 18 | 0 | 0 | 62 | 0.29 | 0.71 | 0.14 | 0.26 |
| 16 | 18 | 33 | 14 | 0 | 0 | 65 | 0.29 | 0.66 | 0.13 | 0.28 |
| 17 | 20 | 33 | 11 | 0 | 0 | 64 | 0.29 | 0.68 | 0.13 | 0.26 |
| 18 | 16 | 34 | 20 | 0 | 0 | 70 | 0.28 | 0.62 | 0.13 | 0.25 |
| 19 | 17 | 28 | 18 | 0 | 0 | 63 | 0.28 | 0.6 | 0.13 | 0.26 |
| 20 | 16 | 37 | 15 | 0 | 0 | 68 | 0.29 | 0.7 | 0.13 | 0.25 |

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

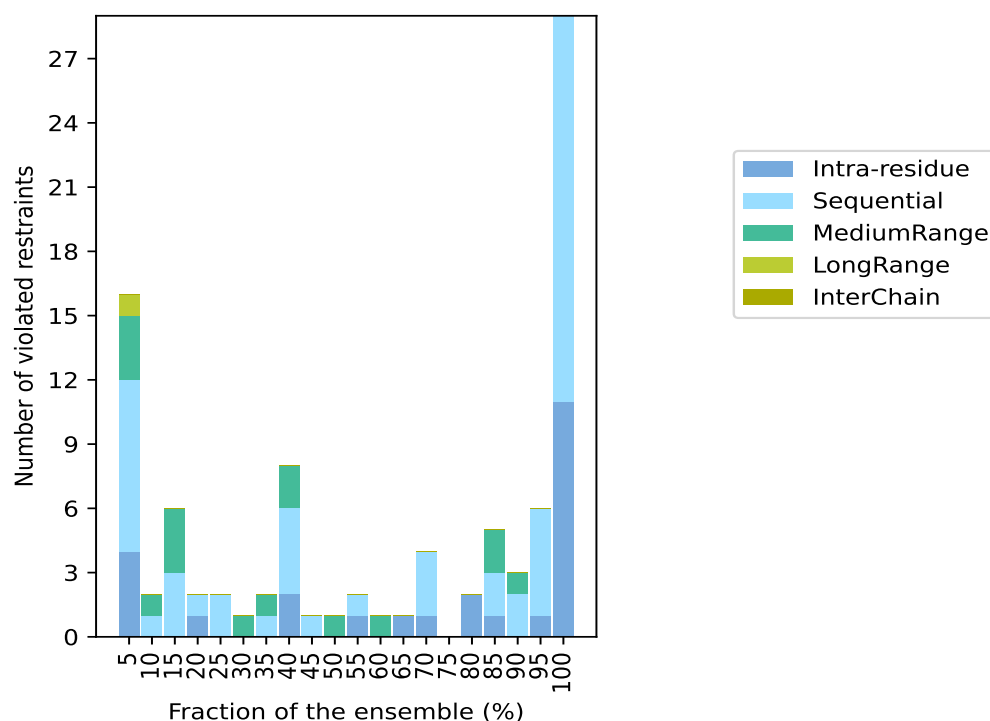
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 363(IR:93, SQ:156, MR:111, LR:3, IC:0) restraints are not 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 | % |
| 4 | 8 | 3 | 1 | 0 | 16 | 1 | 5.0 |
| 0 | 1 | 1 | 0 | 0 | 2 | 2 | 10.0 |
| 0 | 3 | 3 | 0 | 0 | 6 | 3 | 15.0 |
| 1 | 1 | 0 | 0 | 0 | 2 | 4 | 20.0 |
| 0 | 2 | 0 | 0 | 0 | 2 | 5 | 25.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 6 | 30.0 |
| 0 | 1 | 1 | 0 | 0 | 2 | 7 | 35.0 |
| 2 | 4 | 2 | 0 | 0 | 8 | 8 | 40.0 |
| 0 | 1 | 0 | 0 | 0 | 1 | 9 | 45.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 10 | 50.0 |
| 1 | 1 | 0 | 0 | 0 | 2 | 11 | 55.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 12 | 60.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 13 | 65.0 |
| 1 | 3 | 0 | 0 | 0 | 4 | 14 | 70.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 15 | 75.0 |
| 2 | 0 | 0 | 0 | 0 | 2 | 16 | 80.0 |
| 1 | 2 | 2 | 0 | 0 | 5 | 17 | 85.0 |
| 0 | 2 | 1 | 0 | 0 | 3 | 18 | 90.0 |
| 1 | 5 | 0 | 0 | 0 | 6 | 19 | 95.0 |
| 11 | 18 | 0 | 0 | 0 | 29 | 20 | 100.0 |

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

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

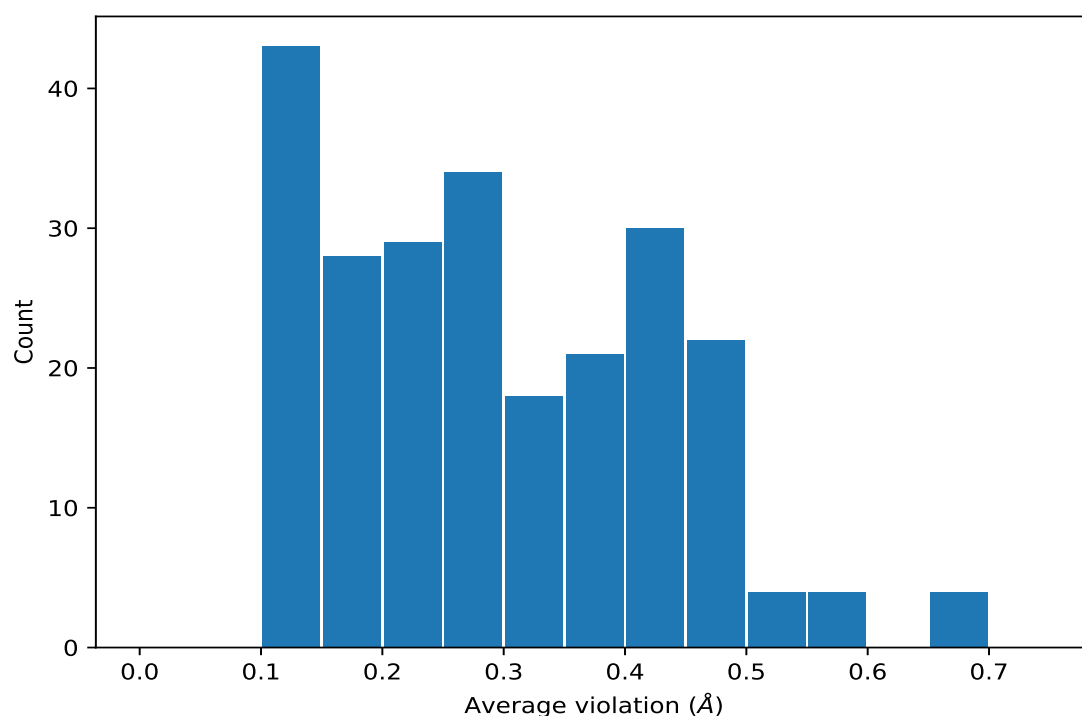
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|---------|--------------|----------------|---------------------|----------|---------------------|------------|
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 20 | 0.67 | 0.07 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 20 | 0.67 | 0.07 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 20 | 0.67 | 0.07 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 20 | 0.67 | 0.07 | 0.68 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 20 | 0.57 | 0.01 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 20 | 0.57 | 0.01 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 20 | 0.57 | 0.01 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 20 | 0.57 | 0.01 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 20 | 0.54 | 0.03 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 20 | 0.54 | 0.03 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 20 | 0.54 | 0.03 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 20 | 0.54 | 0.03 | 0.53 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 20 | 0.47 | 0.03 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 20 | 0.47 | 0.03 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 20 | 0.47 | 0.03 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 20 | 0.47 | 0.03 | 0.46 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 20 | 0.46 | 0.02 | 0.48 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 20 | 0.46 | 0.02 | 0.46 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 20 | 0.45 | 0.12 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 20 | 0.45 | 0.12 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 20 | 0.45 | 0.12 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 20 | 0.45 | 0.12 | 0.5 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 20 | 0.45 | 0.02 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 20 | 0.45 | 0.02 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 20 | 0.45 | 0.02 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 20 | 0.45 | 0.02 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 20 | 0.45 | 0.02 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 20 | 0.45 | 0.02 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 20 | 0.42 | 0.08 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 20 | 0.42 | 0.08 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 20 | 0.42 | 0.08 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 20 | 0.42 | 0.08 | 0.44 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 20 | 0.4 | 0.08 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 20 | 0.4 | 0.08 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 20 | 0.4 | 0.08 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 20 | 0.4 | 0.08 | 0.4 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 20 | 0.4 | 0.08 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 20 | 0.4 | 0.08 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 20 | 0.4 | 0.08 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 20 | 0.4 | 0.08 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 20 | 0.38 | 0.03 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 20 | 0.38 | 0.03 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 20 | 0.38 | 0.03 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 20 | 0.38 | 0.03 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 20 | 0.38 | 0.03 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 20 | 0.38 | 0.03 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 20 | 0.38 | 0.03 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 20 | 0.38 | 0.03 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 20 | 0.38 | 0.03 | 0.38 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 20 | 0.38 | 0.05 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 20 | 0.38 | 0.05 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 20 | 0.38 | 0.05 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 20 | 0.38 | 0.05 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 20 | 0.38 | 0.05 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 20 | 0.38 | 0.05 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 20 | 0.37 | 0.05 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 20 | 0.37 | 0.05 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 20 | 0.37 | 0.05 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 20 | 0.37 | 0.05 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 20 | 0.37 | 0.05 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 20 | 0.37 | 0.05 | 0.38 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 20 | 0.35 | 0.01 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 20 | 0.31 | 0.05 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 20 | 0.31 | 0.05 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 20 | 0.31 | 0.05 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 20 | 0.31 | 0.05 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 20 | 0.31 | 0.05 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 20 | 0.31 | 0.05 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 20 | 0.31 | 0.08 | 0.31 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 20 | 0.31 | 0.08 | 0.31 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 20 | 0.31 | 0.08 | 0.31 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 20 | 0.31 | 0.08 | 0.31 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 20 | 0.3 | 0.07 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 20 | 0.3 | 0.07 | 0.34 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 20 | 0.29 | 0.06 | 0.33 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 20 | 0.29 | 0.02 | 0.29 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 20 | 0.29 | 0.04 | 0.3 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 20 | 0.28 | 0.07 | 0.26 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 20 | 0.28 | 0.07 | 0.26 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 20 | 0.28 | 0.09 | 0.27 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 20 | 0.26 | 0.03 | 0.25 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 20 | 0.24 | 0.03 | 0.25 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 20 | 0.22 | 0.02 | 0.23 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 20 | 0.22 | 0.02 | 0.22 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 20 | 0.18 | 0.03 | 0.18 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 20 | 0.18 | 0.03 | 0.18 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 20 | 0.17 | 0.02 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 20 | 0.14 | 0.02 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 20 | 0.14 | 0.02 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 20 | 0.14 | 0.02 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 20 | 0.14 | 0.02 | 0.14 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 19 | 0.42 | 0.13 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 19 | 0.42 | 0.13 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 19 | 0.42 | 0.13 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 19 | 0.42 | 0.13 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 19 | 0.42 | 0.13 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 19 | 0.42 | 0.13 | 0.45 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 19 | 0.28 | 0.07 | 0.28 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 19 | 0.27 | 0.05 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 19 | 0.27 | 0.05 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 19 | 0.27 | 0.05 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 19 | 0.27 | 0.05 | 0.29 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 19 | 0.25 | 0.09 | 0.23 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 19 | 0.15 | 0.03 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 19 | 0.15 | 0.03 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 19 | 0.15 | 0.03 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 19 | 0.15 | 0.03 | 0.15 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 19 | 0.13 | 0.01 | 0.13 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 18 | 0.25 | 0.07 | 0.26 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 18 | 0.22 | 0.03 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 18 | 0.22 | 0.03 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 18 | 0.22 | 0.03 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 18 | 0.22 | 0.03 | 0.23 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 18 | 0.21 | 0.04 | 0.22 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 18 | 0.2 | 0.04 | 0.2 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 18 | 0.2 | 0.04 | 0.2 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 18 | 0.2 | 0.04 | 0.2 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 18 | 0.2 | 0.04 | 0.2 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 18 | 0.2 | 0.04 | 0.2 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 18 | 0.2 | 0.04 | 0.2 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 17 | 0.49 | 0.14 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 17 | 0.49 | 0.14 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 17 | 0.49 | 0.14 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 17 | 0.49 | 0.14 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 17 | 0.49 | 0.14 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 17 | 0.49 | 0.14 | 0.53 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 17 | 0.23 | 0.08 | 0.22 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 17 | 0.2 | 0.07 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 17 | 0.2 | 0.07 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 17 | 0.2 | 0.07 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 17 | 0.2 | 0.07 | 0.21 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 17 | 0.16 | 0.06 | 0.15 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 17 | 0.16 | 0.02 | 0.16 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 16 | 0.29 | 0.02 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 16 | 0.29 | 0.02 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 16 | 0.29 | 0.02 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 16 | 0.29 | 0.02 | 0.29 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 16 | 0.22 | 0.03 | 0.23 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 16 | 0.2 | 0.03 | 0.2 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 16 | 0.2 | 0.04 | 0.21 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 16 | 0.11 | 0.01 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 16 | 0.11 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 16 | 0.11 | 0.01 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 16 | 0.11 | 0.01 | 0.11 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 15 | 0.24 | 0.06 | 0.24 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 14 | 0.41 | 0.13 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 14 | 0.41 | 0.13 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 14 | 0.41 | 0.13 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 14 | 0.41 | 0.13 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 14 | 0.41 | 0.13 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 14 | 0.41 | 0.13 | 0.44 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 14 | 0.33 | 0.01 | 0.34 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 14 | 0.26 | 0.05 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 14 | 0.26 | 0.05 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 14 | 0.26 | 0.05 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 14 | 0.26 | 0.05 | 0.26 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 14 | 0.25 | 0.1 | 0.29 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 14 | 0.25 | 0.1 | 0.29 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 14 | 0.25 | 0.1 | 0.29 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 14 | 0.25 | 0.1 | 0.29 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 14 | 0.25 | 0.02 | 0.25 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 13 | 0.3 | 0.17 | 0.18 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 13 | 0.3 | 0.17 | 0.18 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 12 | 0.28 | 0.15 | 0.25 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 11 | 0.16 | 0.03 | 0.16 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 11 | 0.14 | 0.03 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 11 | 0.14 | 0.03 | 0.13 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 10 | 0.29 | 0.05 | 0.31 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 10 | 0.29 | 0.05 | 0.31 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 9 | 0.23 | 0.1 | 0.21 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 9 | 0.22 | 0.03 | 0.22 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 8 | 0.33 | 0.14 | 0.39 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 8 | 0.33 | 0.14 | 0.39 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 8 | 0.33 | 0.13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 8 | 0.33 | 0.13 | 0.34 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 8 | 0.33 | 0.13 | 0.34 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 8 | 0.33 | 0.13 | 0.34 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 8 | 0.21 | 0.09 | 0.18 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 8 | 0.19 | 0.06 | 0.17 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 8 | 0.19 | 0.06 | 0.17 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 8 | 0.19 | 0.06 | 0.17 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 8 | 0.19 | 0.06 | 0.17 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 8 | 0.17 | 0.04 | 0.18 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 8 | 0.16 | 0.05 | 0.16 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 8 | 0.16 | 0.05 | 0.16 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 8 | 0.16 | 0.05 | 0.16 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 8 | 0.16 | 0.05 | 0.16 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 8 | 0.16 | 0.04 | 0.15 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 8 | 0.16 | 0.04 | 0.15 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 8 | 0.16 | 0.03 | 0.17 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 8 | 0.12 | 0.01 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 8 | 0.12 | 0.01 | 0.12 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 7 | 0.43 | 0.07 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 7 | 0.43 | 0.07 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 7 | 0.43 | 0.07 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 7 | 0.43 | 0.07 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 7 | 0.43 | 0.07 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 7 | 0.43 | 0.07 | 0.46 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 7 | 0.18 | 0.05 | 0.17 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 6 | 0.18 | 0.03 | 0.2 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 6 | 0.17 | 0.03 | 0.16 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 6 | 0.15 | 0.03 | 0.15 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 5 | 0.24 | 0.03 | 0.22 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 5 | 0.24 | 0.03 | 0.22 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 5 | 0.13 | 0.03 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 5 | 0.13 | 0.03 | 0.11 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG2 | 4 | 0.15 | 0.07 | 0.12 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG3 | 4 | 0.15 | 0.07 | 0.12 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 4 | 0.14 | 0.01 | 0.14 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 4 | 0.14 | 0.01 | 0.14 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 4 | 0.14 | 0.01 | 0.14 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 4 | 0.14 | 0.01 | 0.14 |
| (1,7) | 1:26:A:PHE:H | 1:22:A:ARG:O | 3 | 0.22 | 0.02 | 0.22 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 3 | 0.18 | 0.06 | 0.19 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 3 | 0.18 | 0.06 | 0.19 |
| (2,333) | 1:15:A:THR:H | 1:18:A:CYS:H | 3 | 0.17 | 0.03 | 0.15 |

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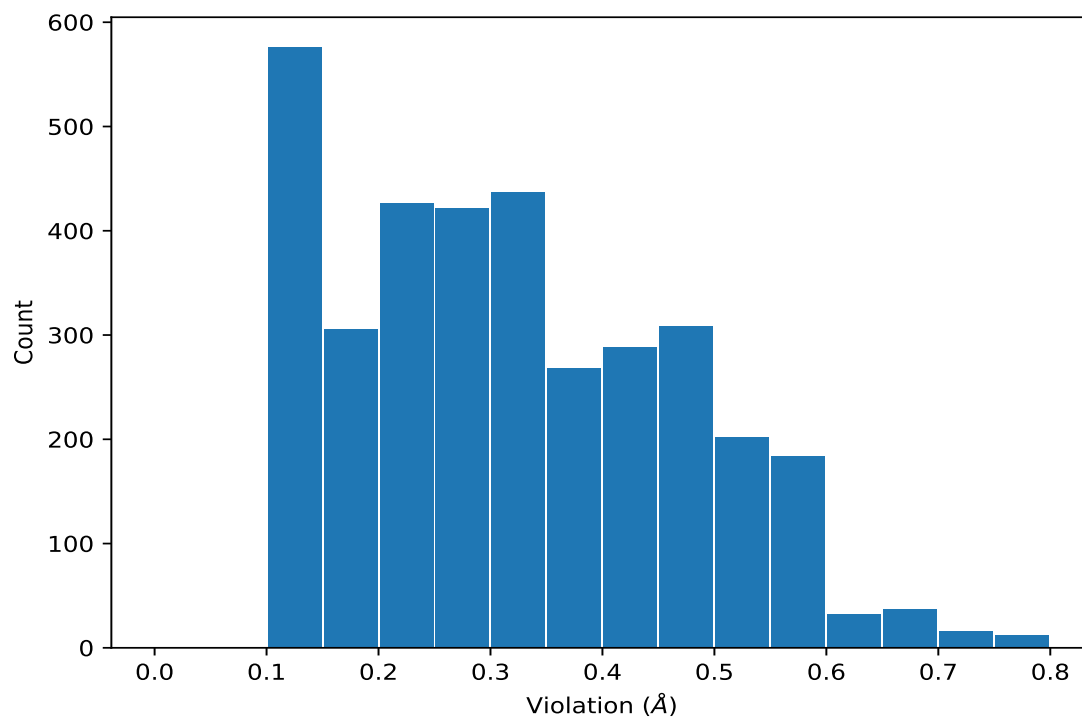
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|--------------|----------------|---------------------|----------|---------------------|------------|
| (2,385) | 1:32:A:ASN:H | 1:30:A:SER:HA | 3 | 0.17 | 0.06 | 0.14 |
| (2,400) | 1:36:A:ALA:H | 1:34:A:PHE:HA | 3 | 0.14 | 0.03 | 0.12 |
| (2,131) | 1:16:A:ALA:H | 1:17:A:THR:H | 3 | 0.13 | 0.02 | 0.15 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 3 | 0.12 | 0.0 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 3 | 0.12 | 0.0 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 3 | 0.12 | 0.0 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 3 | 0.12 | 0.0 | 0.12 |
| (1,18) | 1:59:A:ARG:H | 1:55:A:GLU:O | 2 | 0.19 | 0.01 | 0.19 |
| (2,160) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 2 | 0.19 | 0.03 | 0.19 |
| (2,160) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 2 | 0.19 | 0.03 | 0.19 |
| (2,373) | 1:30:A:SER:H | 1:26:A:PHE:HA | 2 | 0.11 | 0.01 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 10 | 0.79 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 10 | 0.79 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 10 | 0.79 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 10 | 0.79 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 9 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 9 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 9 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 9 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 14 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 14 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 14 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 14 | 0.77 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 7 | 0.73 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 7 | 0.73 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 7 | 0.73 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 7 | 0.73 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 13 | 0.72 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 13 | 0.72 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 13 | 0.72 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 13 | 0.72 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 11 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 11 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 11 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 11 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 15 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 15 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 15 | 0.71 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 15 | 0.71 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 8 | 0.7 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 8 | 0.7 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 8 | 0.7 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 8 | 0.7 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 8 | 0.7 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 8 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 3 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 3 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 3 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 3 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 20 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 20 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 20 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 20 | 0.7 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 2 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 2 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 2 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 2 | 0.68 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 17 | 0.68 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 17 | 0.68 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 17 | 0.68 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 17 | 0.68 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 17 | 0.68 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 17 | 0.68 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 17 | 0.67 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 17 | 0.67 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 17 | 0.67 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 17 | 0.67 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 8 | 0.66 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 16 | 0.66 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 16 | 0.66 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 16 | 0.66 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 16 | 0.66 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 8 | 0.65 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 8 | 0.65 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 8 | 0.65 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 8 | 0.65 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 12 | 0.64 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 12 | 0.64 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 12 | 0.64 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 12 | 0.64 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 20 | 0.63 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 20 | 0.63 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 20 | 0.63 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 20 | 0.63 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 20 | 0.63 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 20 | 0.63 |
| (2,410) | 1:52:A:ASN:H | 1:55:A:GLU:HG2 | 9 | 0.62 |
| (2,410) | 1:52:A:ASN:H | 1:55:A:GLU:HG2 | 9 | 0.62 |
| (2,410) | 1:52:A:ASN:H | 1:55:A:GLU:HG3 | 9 | 0.62 |
| (2,410) | 1:52:A:ASN:H | 1:55:A:GLU:HG3 | 9 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 15 | 0.62 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 15 | 0.62 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 15 | 0.62 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 15 | 0.62 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 15 | 0.62 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 15 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 1 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 1 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 1 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 1 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 18 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 18 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 18 | 0.62 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 18 | 0.62 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 7 | 0.62 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 7 | 0.62 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 7 | 0.62 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 7 | 0.62 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 12 | 0.6 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 12 | 0.6 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 12 | 0.6 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 12 | 0.6 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 12 | 0.6 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 12 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 4 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 4 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 4 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 4 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 19 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 19 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 19 | 0.6 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 19 | 0.6 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 13 | 0.59 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 13 | 0.59 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 13 | 0.59 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 13 | 0.59 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 13 | 0.59 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 13 | 0.59 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 8 | 0.59 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 8 | 0.59 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 8 | 0.59 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 8 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 15 | 0.59 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 15 | 0.59 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 15 | 0.59 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 15 | 0.59 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 4 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 4 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 4 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 4 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 4 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 4 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 7 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 7 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 7 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 7 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 7 | 0.58 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 7 | 0.58 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 5 | 0.58 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 5 | 0.58 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 5 | 0.58 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 5 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 3 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 3 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 3 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 3 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 10 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 10 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 10 | 0.58 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 10 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 1 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 1 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 1 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 1 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 3 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 3 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 3 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 3 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 8 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 8 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 8 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 8 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 9 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 9 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 9 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 9 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 10 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 10 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 10 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 10 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 15 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 15 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 15 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 15 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 16 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 16 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 16 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 16 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 20 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 20 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 20 | 0.58 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 20 | 0.58 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 6 | 0.57 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG2 | 6 | 0.57 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 6 | 0.57 |
| (2,267) | 1:52:A:ASN:H | 1:51:A:ARG:HG3 | 6 | 0.57 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 9 | 0.57 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 9 | 0.57 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 9 | 0.57 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 9 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 13 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 13 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 13 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 13 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 14 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 14 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 14 | 0.57 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 14 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 4 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 4 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 4 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 4 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 5 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 5 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 5 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 5 | 0.57 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 6 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 6 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 6 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 6 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 7 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 7 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 7 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 7 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 11 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 11 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 11 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 11 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 12 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 12 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 12 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 12 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 14 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 14 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 14 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 14 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 17 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 17 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 17 | 0.57 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 17 | 0.57 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 13 | 0.57 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 13 | 0.57 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 13 | 0.57 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 13 | 0.57 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 13 | 0.57 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 13 | 0.57 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 19 | 0.56 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 19 | 0.56 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 19 | 0.56 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 19 | 0.56 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 17 | 0.56 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 17 | 0.56 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 17 | 0.56 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 17 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 2 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 2 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 2 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 2 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 13 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 13 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 13 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 13 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 18 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 18 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 18 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 18 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 19 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB2 | 19 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 19 | 0.56 |
| (2,97) | 1:57:A:LEU:H | 1:57:A:LEU:HB3 | 19 | 0.56 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 6 | 0.55 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 6 | 0.55 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 6 | 0.55 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 6 | 0.55 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 11 | 0.55 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 11 | 0.55 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 11 | 0.55 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 11 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 7 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 7 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 7 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 7 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 11 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 11 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 11 | 0.55 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 11 | 0.55 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 4 | 0.55 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 4 | 0.55 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 4 | 0.55 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 4 | 0.55 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 4 | 0.55 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 4 | 0.55 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 18 | 0.54 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 18 | 0.54 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 18 | 0.54 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 18 | 0.54 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 18 | 0.54 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 18 | 0.54 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 5 | 0.54 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 5 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 5 | 0.54 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 5 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 3 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 3 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 3 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 3 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 13 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 13 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 13 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 13 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 14 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 14 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 14 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 14 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 15 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 15 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 15 | 0.54 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 15 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 6 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 6 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 6 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 6 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 6 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 6 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 16 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 16 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 16 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 16 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 16 | 0.54 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 16 | 0.54 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 10 | 0.54 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 10 | 0.54 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 10 | 0.54 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 10 | 0.54 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 4 | 0.54 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 4 | 0.54 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 4 | 0.54 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 4 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 10 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 10 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 10 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 10 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 10 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 10 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 14 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 14 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 14 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 14 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 14 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 14 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 15 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 15 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 15 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 15 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 15 | 0.54 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 15 | 0.54 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 2 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 2 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 2 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 2 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 2 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 2 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 11 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 11 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 11 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 11 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 11 | 0.53 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 11 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 10 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 10 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 10 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 10 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 11 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 11 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 11 | 0.53 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 11 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 1 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 1 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 1 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 1 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 4 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 4 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 4 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 4 | 0.53 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 12 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 12 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 12 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 12 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 20 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 20 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 20 | 0.53 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 20 | 0.53 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 3 | 0.53 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 3 | 0.53 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 3 | 0.53 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 3 | 0.53 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 3 | 0.53 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 3 | 0.53 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 19 | 0.52 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 19 | 0.52 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 19 | 0.52 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 19 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 5 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 5 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 5 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 5 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 6 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 6 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 6 | 0.52 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 6 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 3 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 3 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 3 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 3 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 12 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 12 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 12 | 0.52 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 12 | 0.52 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 9 | 0.52 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 9 | 0.52 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 9 | 0.52 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 9 | 0.52 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 9 | 0.52 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 9 | 0.52 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 13 | 0.52 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 13 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 16 | 0.51 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 16 | 0.51 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 16 | 0.51 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 16 | 0.51 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 4 | 0.51 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 4 | 0.51 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 4 | 0.51 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 4 | 0.51 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 8 | 0.51 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 8 | 0.51 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 8 | 0.51 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 8 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 2 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 2 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 2 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 2 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 9 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 9 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 9 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 9 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 18 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 18 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 18 | 0.51 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 18 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 11 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 11 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 11 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 11 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 11 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 11 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 18 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 18 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 18 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 18 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 18 | 0.51 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 18 | 0.51 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 11 | 0.51 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 11 | 0.51 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 1 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 1 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 1 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 1 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 5 | 0.5 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 5 | 0.5 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 5 | 0.5 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 5 | 0.5 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 5 | 0.5 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 5 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 8 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 8 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 8 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 8 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 16 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 16 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 16 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 16 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 19 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG2 | 19 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 19 | 0.5 |
| (2,99) | 1:58:A:LYS:H | 1:58:A:LYS:HG3 | 19 | 0.5 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 7 | 0.5 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 7 | 0.5 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 7 | 0.5 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 7 | 0.5 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 2 | 0.5 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 2 | 0.5 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 2 | 0.5 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 2 | 0.5 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 18 | 0.49 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 18 | 0.49 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 18 | 0.49 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 18 | 0.49 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 7 | 0.49 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 15 | 0.49 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 19 | 0.49 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 19 | 0.49 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 18 | 0.49 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 18 | 0.49 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 18 | 0.49 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 18 | 0.49 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 18 | 0.49 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 18 | 0.49 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 8 | 0.49 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 8 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 8 | 0.49 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 8 | 0.49 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 8 | 0.49 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 8 | 0.49 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 4 | 0.49 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 4 | 0.49 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 6 | 0.48 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 6 | 0.48 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 6 | 0.48 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 6 | 0.48 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 6 | 0.48 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 6 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 4 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 4 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 4 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 4 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 8 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 8 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 8 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 8 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 12 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 12 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 12 | 0.48 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 12 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 3 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 4 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 9 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 10 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 11 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 13 | 0.48 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 14 | 0.48 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 1 | 0.48 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 4 | 0.48 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 5 | 0.48 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 13 | 0.48 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 8 | 0.48 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 8 | 0.48 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 8 | 0.48 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 8 | 0.48 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 8 | 0.48 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 8 | 0.48 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 17 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 17 | 0.48 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 17 | 0.48 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 17 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 8 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 8 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 8 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 8 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 18 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 18 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 18 | 0.48 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 18 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 5 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 5 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 5 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 5 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 5 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 5 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 6 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 6 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 6 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 6 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 6 | 0.48 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 6 | 0.48 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 9 | 0.48 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 9 | 0.48 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 9 | 0.48 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 9 | 0.48 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 20 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 2 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 2 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 2 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 2 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 2 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 2 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 3 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 3 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 3 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 3 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 3 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 3 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 8 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 8 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 8 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 8 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 8 | 0.47 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 8 | 0.47 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 18 | 0.47 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 18 | 0.47 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 18 | 0.47 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 18 | 0.47 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 1 | 0.47 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 18 | 0.47 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 6 | 0.47 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 11 | 0.47 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 15 | 0.47 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 16 | 0.47 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 5 | 0.47 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 5 | 0.47 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 5 | 0.47 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 5 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 5 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 5 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 5 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 5 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 6 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 6 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 6 | 0.47 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 6 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 16 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 16 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 16 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 16 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 16 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 16 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 20 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 20 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 20 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 20 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 20 | 0.47 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 20 | 0.47 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 5 | 0.46 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 5 | 0.46 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 5 | 0.46 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 5 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 5 | 0.46 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 5 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 1 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 1 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 1 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 1 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 1 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 1 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 10 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 10 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 10 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 10 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 10 | 0.46 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 10 | 0.46 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 8 | 0.46 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 7 | 0.46 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 8 | 0.46 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 9 | 0.46 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 10 | 0.46 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 14 | 0.46 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 18 | 0.46 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 5 | 0.46 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 5 | 0.46 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 5 | 0.46 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 5 | 0.46 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 5 | 0.46 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 5 | 0.46 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 20 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 1 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 1 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 1 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 1 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 10 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 10 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 10 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 10 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 14 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 14 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 14 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 14 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 16 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 16 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 16 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 16 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 20 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 20 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 20 | 0.46 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 20 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 1 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 1 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 1 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 1 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 1 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 1 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 2 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 2 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 2 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 2 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 2 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 2 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 18 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 18 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 18 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 18 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 18 | 0.46 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 18 | 0.46 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 4 | 0.46 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 4 | 0.46 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 4 | 0.46 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 4 | 0.46 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 1 | 0.46 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 1 | 0.46 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 16 | 0.46 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 16 | 0.46 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 20 | 0.45 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 20 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 1 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 1 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 1 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 1 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 3 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 3 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 3 | 0.45 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 3 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 5 | 0.45 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 6 | 0.45 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 16 | 0.45 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 3 | 0.45 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 19 | 0.45 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 19 | 0.45 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 19 | 0.45 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 19 | 0.45 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 19 | 0.45 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 19 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 2 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 2 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 2 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 2 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 9 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 9 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 9 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 9 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 15 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 15 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 15 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 15 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 17 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 17 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 17 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 17 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 19 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 19 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 19 | 0.45 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 19 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 3 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 3 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 3 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 3 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 3 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 3 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 9 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 9 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 9 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 9 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 9 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 9 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 12 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 12 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 12 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 12 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 12 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 12 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 14 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 14 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 14 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 14 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 14 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 14 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 17 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 17 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 17 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 17 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 17 | 0.45 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 17 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 10 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 10 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 10 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 10 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 17 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 17 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 17 | 0.45 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 17 | 0.45 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 18 | 0.45 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 18 | 0.45 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 18 | 0.45 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 18 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 1 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 1 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 1 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 1 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 1 | 0.45 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 1 | 0.45 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 13 | 0.45 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 13 | 0.45 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 6 | 0.45 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 6 | 0.45 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 1 | 0.44 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 1 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 1 | 0.44 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 1 | 0.44 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 1 | 0.44 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 1 | 0.44 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 11 | 0.44 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 11 | 0.44 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 11 | 0.44 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 11 | 0.44 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 8 | 0.44 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 8 | 0.44 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 8 | 0.44 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 8 | 0.44 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 10 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 12 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 12 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 12 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 12 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 12 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 12 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 17 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 17 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 17 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 17 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 17 | 0.44 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 17 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 17 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 17 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 17 | 0.44 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 17 | 0.44 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 20 | 0.44 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 20 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 3 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 3 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 3 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 3 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 3 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 3 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 9 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 9 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 9 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 9 | 0.44 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 9 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 9 | 0.44 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 12 | 0.44 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 12 | 0.44 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 12 | 0.44 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 12 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 11 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 11 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 11 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 11 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 13 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG2 | 13 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 13 | 0.44 |
| (2,78) | 1:51:A:ARG:H | 1:51:A:ARG:HG3 | 13 | 0.44 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 15 | 0.44 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 15 | 0.44 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 15 | 0.44 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 15 | 0.44 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 11 | 0.44 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 11 | 0.44 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 2 | 0.43 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 2 | 0.43 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 19 | 0.43 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 19 | 0.43 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 19 | 0.43 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 19 | 0.43 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 2 | 0.43 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 6 | 0.43 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 6 | 0.43 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 6 | 0.43 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 6 | 0.43 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 6 | 0.43 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 6 | 0.43 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 15 | 0.43 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 15 | 0.43 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 15 | 0.43 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 15 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 4 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 4 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 4 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 4 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 4 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 7 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 7 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 7 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 7 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 7 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 7 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 11 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 11 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 11 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 11 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 11 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 11 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 15 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 15 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 15 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 15 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 15 | 0.43 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 15 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 12 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 12 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 12 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 12 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 20 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 20 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 20 | 0.43 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 20 | 0.43 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 19 | 0.42 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 5 | 0.42 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 5 | 0.42 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 5 | 0.42 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 5 | 0.42 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 8 | 0.42 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 8 | 0.42 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 8 | 0.42 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 8 | 0.42 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 9 | 0.42 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 18 | 0.42 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 18 | 0.42 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 18 | 0.42 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 18 | 0.42 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 18 | 0.42 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 18 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 8 | 0.42 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 8 | 0.42 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 8 | 0.42 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 8 | 0.42 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 12 | 0.42 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 2 | 0.42 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 8 | 0.42 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 8 | 0.42 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 8 | 0.42 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 8 | 0.42 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 8 | 0.42 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 8 | 0.42 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 1 | 0.42 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 1 | 0.42 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 1 | 0.42 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 1 | 0.42 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 1 | 0.42 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 1 | 0.42 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 20 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 10 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 10 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 10 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 10 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 10 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 10 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 19 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 19 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 19 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 19 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 19 | 0.42 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 19 | 0.42 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 5 | 0.42 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 5 | 0.42 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 5 | 0.42 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 5 | 0.42 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 5 | 0.42 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 5 | 0.42 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 4 | 0.42 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 4 | 0.42 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 11 | 0.41 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 13 | 0.41 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 13 | 0.41 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 13 | 0.41 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 13 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 7 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 7 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 7 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 7 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 10 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 10 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 10 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 10 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 11 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 11 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 11 | 0.41 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 11 | 0.41 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 1 | 0.41 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 1 | 0.41 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 1 | 0.41 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 1 | 0.41 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 15 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 11 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 11 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 11 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 11 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 11 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 11 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 19 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 19 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 19 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 19 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 19 | 0.41 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 19 | 0.41 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 12 | 0.41 |
| (2,220) | 1:33:A:ASN:H | 1:32:A:ASN:HA | 17 | 0.41 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 7 | 0.41 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 7 | 0.41 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 7 | 0.41 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 7 | 0.41 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 7 | 0.41 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 7 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 6 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 6 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 6 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 6 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 7 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 7 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 7 | 0.41 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 7 | 0.41 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG11 | 13 | 0.41 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG12 | 13 | 0.41 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG13 | 13 | 0.41 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG21 | 13 | 0.41 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG22 | 13 | 0.41 |
| (2,42) | 1:28:A:VAL:H | 1:28:A:VAL:HG23 | 13 | 0.41 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 14 | 0.41 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 14 | 0.41 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 14 | 0.41 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 14 | 0.41 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 13 | 0.41 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 13 | 0.41 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 13 | 0.41 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 13 | 0.41 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 14 | 0.4 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 14 | 0.4 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 14 | 0.4 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 14 | 0.4 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 14 | 0.4 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 14 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 1 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 1 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 1 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 1 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 6 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 6 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 6 | 0.4 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 6 | 0.4 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 3 | 0.4 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 16 | 0.4 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 16 | 0.4 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 16 | 0.4 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 16 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 1 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 1 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 1 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 1 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 1 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 1 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 8 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 8 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 8 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 8 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 8 | 0.4 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 8 | 0.4 |
| (2,221) | 1:34:A:PHE:H | 1:33:A:ASN:HA | 17 | 0.4 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 2 | 0.4 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 2 | 0.4 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 2 | 0.4 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 2 | 0.4 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 2 | 0.4 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 2 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 14 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 14 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 14 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 14 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 16 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 16 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 16 | 0.4 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 16 | 0.4 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 7 | 0.4 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 7 | 0.4 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 7 | 0.4 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 7 | 0.4 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 6 | 0.4 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 6 | 0.4 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 6 | 0.4 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 6 | 0.4 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 6 | 0.4 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 6 | 0.4 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 20 | 0.39 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 10 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 4 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 4 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 4 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 4 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 17 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 17 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 17 | 0.39 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 17 | 0.39 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 18 | 0.39 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 18 | 0.39 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 18 | 0.39 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 18 | 0.39 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 20 | 0.39 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 20 | 0.39 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 20 | 0.39 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 20 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 2 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 2 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 2 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 2 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 2 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 2 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 4 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 4 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 4 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 4 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 4 | 0.39 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 4 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 2 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 2 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 2 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 2 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 7 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 7 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 7 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 7 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 11 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 11 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 11 | 0.39 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 11 | 0.39 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 5 | 0.39 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 5 | 0.39 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 5 | 0.39 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 5 | 0.39 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 5 | 0.39 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 5 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 3 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 3 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 3 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 3 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 3 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 3 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 10 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 10 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 10 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 10 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 10 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 10 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 12 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 12 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 12 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 12 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 12 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 12 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 14 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 14 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 14 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 14 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 14 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 14 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 16 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 16 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 16 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 16 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 16 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 16 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 18 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 18 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 18 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 18 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 18 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 18 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 20 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 20 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 20 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 20 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 20 | 0.39 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 20 | 0.39 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 15 | 0.39 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 15 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 15 | 0.39 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 15 | 0.39 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 10 | 0.39 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 10 | 0.39 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 10 | 0.39 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 10 | 0.39 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 1 | 0.39 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 1 | 0.39 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 16 | 0.39 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 16 | 0.39 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 7 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 13 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 13 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 13 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 13 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 16 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 16 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 16 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 16 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 18 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 18 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 18 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 18 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 4 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 5 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 5 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 5 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 5 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 7 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 11 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 17 | 0.38 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 19 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 13 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 13 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 13 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 13 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 13 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 13 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 20 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 20 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 20 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 20 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 20 | 0.38 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 20 | 0.38 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 10 | 0.38 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 10 | 0.38 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 10 | 0.38 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 10 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 5 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 5 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 5 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 5 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 16 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 16 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 16 | 0.38 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 16 | 0.38 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 16 | 0.38 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 16 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 4 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 4 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 4 | 0.38 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 4 | 0.38 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 7 | 0.38 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 7 | 0.38 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 7 | 0.38 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 7 | 0.38 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 7 | 0.38 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 7 | 0.38 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 6 | 0.38 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 6 | 0.38 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 17 | 0.38 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 3 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 3 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 3 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 3 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 12 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 12 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 12 | 0.37 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 12 | 0.37 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 2 | 0.37 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 14 | 0.37 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 14 | 0.37 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 14 | 0.37 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 14 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 6 | 0.37 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 6 | 0.37 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 6 | 0.37 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 6 | 0.37 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 6 | 0.37 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 6 | 0.37 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 11 | 0.37 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 19 | 0.37 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 14 | 0.37 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 14 | 0.37 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 7 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 1 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 1 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 1 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 1 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 3 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 3 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 3 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 3 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 9 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 9 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 9 | 0.37 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 9 | 0.37 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 6 | 0.37 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 6 | 0.37 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 6 | 0.37 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 6 | 0.37 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 1 | 0.37 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 1 | 0.37 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 1 | 0.37 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 1 | 0.37 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 16 | 0.36 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 16 | 0.36 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 16 | 0.36 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 16 | 0.36 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 16 | 0.36 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 16 | 0.36 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 8 | 0.36 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 8 | 0.36 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 8 | 0.36 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 8 | 0.36 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 19 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 19 | 0.36 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 19 | 0.36 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 19 | 0.36 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 12 | 0.36 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 14 | 0.36 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 18 | 0.36 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 18 | 0.36 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 18 | 0.36 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 18 | 0.36 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 6 | 0.36 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 6 | 0.36 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 6 | 0.36 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 6 | 0.36 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 9 | 0.36 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 9 | 0.36 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 9 | 0.36 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 9 | 0.36 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 9 | 0.36 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 9 | 0.36 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 10 | 0.36 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 13 | 0.36 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 3 | 0.36 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 3 | 0.36 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 20 | 0.36 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 20 | 0.36 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 20 | 0.36 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 20 | 0.36 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 20 | 0.36 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 20 | 0.36 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 1 | 0.36 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 5 | 0.36 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 8 | 0.36 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 16 | 0.36 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 20 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 3 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 3 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 3 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 3 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 11 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 11 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 11 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 13 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 13 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 13 | 0.36 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 13 | 0.36 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 11 | 0.36 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 11 | 0.36 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 11 | 0.36 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 11 | 0.36 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 15 | 0.35 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 9 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 2 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 2 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 2 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 2 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 14 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 14 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 14 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 14 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 15 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 15 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 15 | 0.35 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 15 | 0.35 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 16 | 0.35 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 16 | 0.35 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 16 | 0.35 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 16 | 0.35 |
| (2,297) | 1:57:A:LEU:H | 1:57:A:LEU:HG | 13 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 5 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 5 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 5 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 5 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 5 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 5 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 6 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 6 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 6 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 6 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 6 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 6 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 16 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 16 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 16 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 16 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 16 | 0.35 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 16 | 0.35 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 9 | 0.35 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 9 | 0.35 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 9 | 0.35 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 9 | 0.35 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 20 | 0.35 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 20 | 0.35 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 20 | 0.35 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 20 | 0.35 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 5 | 0.35 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 5 | 0.35 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 5 | 0.35 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 5 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 1 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 1 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 1 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 1 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 1 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 1 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 7 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 7 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 7 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 7 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 7 | 0.35 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 7 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 1 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 1 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 5 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 5 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 6 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 6 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 18 | 0.35 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 18 | 0.35 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 14 | 0.35 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 14 | 0.35 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 14 | 0.35 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 14 | 0.35 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 14 | 0.35 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 14 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 2 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 2 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 2 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 2 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 13 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 13 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 13 | 0.35 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 13 | 0.35 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 6 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 2 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 3 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 4 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 7 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 9 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 12 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 14 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 15 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 17 | 0.35 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 18 | 0.35 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 16 | 0.35 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 16 | 0.35 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 16 | 0.35 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 16 | 0.35 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 16 | 0.35 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 16 | 0.35 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 10 | 0.34 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 10 | 0.34 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 9 | 0.34 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 14 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 9 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 9 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 9 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 9 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 20 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB2 | 20 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 20 | 0.34 |
| (2,320) | 1:63:A:ASN:H | 1:62:A:LEU:HB3 | 20 | 0.34 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 12 | 0.34 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 12 | 0.34 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 6 | 0.34 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 6 | 0.34 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 6 | 0.34 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 6 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 3 | 0.34 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 3 | 0.34 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 3 | 0.34 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 3 | 0.34 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 3 | 0.34 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 3 | 0.34 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 8 | 0.34 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 8 | 0.34 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 8 | 0.34 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 8 | 0.34 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 2 | 0.34 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 2 | 0.34 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 2 | 0.34 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 2 | 0.34 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 2 | 0.34 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 2 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 7 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 7 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 8 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 8 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 12 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 12 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 17 | 0.34 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 17 | 0.34 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 2 | 0.34 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 9 | 0.34 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 14 | 0.34 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 18 | 0.34 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 18 | 0.34 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 18 | 0.34 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 18 | 0.34 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 15 | 0.34 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 17 | 0.34 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 19 | 0.34 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 10 | 0.34 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 11 | 0.34 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 13 | 0.34 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 19 | 0.34 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 4 | 0.34 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 8 | 0.34 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 10 | 0.34 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 11 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 14 | 0.34 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 15 | 0.34 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 19 | 0.34 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 19 | 0.34 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 19 | 0.34 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 19 | 0.34 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 19 | 0.34 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 15 | 0.33 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 15 | 0.33 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 19 | 0.33 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 19 | 0.33 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 17 | 0.33 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 18 | 0.33 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 18 | 0.33 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 2 | 0.33 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 2 | 0.33 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 2 | 0.33 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 2 | 0.33 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 2 | 0.33 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 2 | 0.33 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 2 | 0.33 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 2 | 0.33 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 5 | 0.33 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 6 | 0.33 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 8 | 0.33 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 6 | 0.33 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 6 | 0.33 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 6 | 0.33 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 6 | 0.33 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 10 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 3 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 3 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 3 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 3 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 3 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 3 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 10 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 10 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 10 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 10 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 10 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 10 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 18 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 18 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 18 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 18 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 18 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 18 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 20 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 20 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 20 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 20 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 20 | 0.33 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 20 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 13 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 13 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 13 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 13 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 13 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 13 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 15 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 15 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 15 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 15 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 15 | 0.33 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 15 | 0.33 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 7 | 0.33 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 3 | 0.33 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 1 | 0.33 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 1 | 0.33 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 1 | 0.33 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 1 | 0.33 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 1 | 0.33 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 1 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 4 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 5 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 7 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 9 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 11 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 12 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 13 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 16 | 0.33 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 18 | 0.33 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 8 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 8 | 0.33 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 8 | 0.33 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 8 | 0.33 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 10 | 0.33 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 13 | 0.33 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 19 | 0.33 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 1 | 0.33 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 3 | 0.33 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 16 | 0.33 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 17 | 0.33 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 18 | 0.33 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 20 | 0.33 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 12 | 0.32 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 12 | 0.32 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 12 | 0.32 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 4 | 0.32 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 17 | 0.32 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 1 | 0.32 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 1 | 0.32 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 16 | 0.32 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 16 | 0.32 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 19 | 0.32 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 19 | 0.32 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 19 | 0.32 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 19 | 0.32 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 6 | 0.32 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB2 | 6 | 0.32 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 6 | 0.32 |
| (2,297) | 1:57:A:LEU:H | 1:58:A:LYS:HB3 | 6 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 9 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 9 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 9 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 9 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 9 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 9 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 15 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 15 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 15 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 15 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 15 | 0.32 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 15 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 13 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 13 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 13 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 13 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 20 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 20 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 20 | 0.32 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 20 | 0.32 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 16 | 0.32 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 16 | 0.32 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 16 | 0.32 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 16 | 0.32 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 16 | 0.32 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 13 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 12 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 12 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 12 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 12 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 12 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 12 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 14 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 14 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 14 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 14 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 14 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 14 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 16 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 16 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 16 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 16 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 16 | 0.32 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 16 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 4 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 4 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 4 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 4 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 4 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 4 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 17 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 17 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 17 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 17 | 0.32 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 17 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 17 | 0.32 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 4 | 0.32 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 17 | 0.32 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 2 | 0.32 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 2 | 0.32 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 12 | 0.32 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 17 | 0.32 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 20 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 5 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 5 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 5 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 5 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 19 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 19 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 19 | 0.32 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 19 | 0.32 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 11 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 1 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 1 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 1 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 1 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 16 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 16 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 16 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 16 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 16 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 18 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 18 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 18 | 0.32 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 18 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 5 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 5 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 5 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 5 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 6 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 6 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 6 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 6 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 19 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 19 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 19 | 0.32 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 19 | 0.32 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 9 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 6 | 0.31 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 3 | 0.31 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 3 | 0.31 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 17 | 0.31 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 17 | 0.31 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 7 | 0.31 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 9 | 0.31 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 10 | 0.31 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 10 | 0.31 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 10 | 0.31 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 10 | 0.31 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 10 | 0.31 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 10 | 0.31 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 18 | 0.31 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 18 | 0.31 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 18 | 0.31 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 18 | 0.31 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 9 | 0.31 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 9 | 0.31 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 9 | 0.31 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 9 | 0.31 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 4 | 0.31 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 4 | 0.31 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 4 | 0.31 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 4 | 0.31 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 7 | 0.31 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 7 | 0.31 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 7 | 0.31 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 7 | 0.31 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 7 | 0.31 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 7 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 3 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 3 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 3 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 3 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 11 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 11 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 11 | 0.31 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 11 | 0.31 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 13 | 0.31 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 13 | 0.31 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 13 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 13 | 0.31 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 2 | 0.31 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 7 | 0.31 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 12 | 0.31 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 14 | 0.31 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 11 | 0.31 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 15 | 0.31 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 19 | 0.31 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 9 | 0.31 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 9 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 1 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 1 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 1 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 1 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 6 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 6 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 6 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 6 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 18 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 18 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 18 | 0.31 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 18 | 0.31 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 15 | 0.31 |
| (2,40) | 1:27:A:LEU:H | 1:27:A:LEU:HG | 6 | 0.31 |
| (2,33) | 1:25:A:ASN:H | 1:25:A:ASN:HB3 | 5 | 0.31 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 13 | 0.3 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 15 | 0.3 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 20 | 0.3 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 20 | 0.3 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 20 | 0.3 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 20 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 1 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 1 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 1 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 1 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 10 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 10 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 10 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 10 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 18 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 18 | 0.3 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 18 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 18 | 0.3 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 1 | 0.3 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 3 | 0.3 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 9 | 0.3 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 20 | 0.3 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 15 | 0.3 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 2 | 0.3 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 4 | 0.3 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 4 | 0.3 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 4 | 0.3 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 4 | 0.3 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 4 | 0.3 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 4 | 0.3 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 7 | 0.3 |
| (2,19) | 1:21:A:GLN:H | 1:21:A:GLN:HG2 | 8 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 3 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 3 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 3 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 3 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 14 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 14 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 14 | 0.3 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 14 | 0.3 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 1 | 0.3 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 1 | 0.29 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 2 | 0.29 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 18 | 0.29 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 18 | 0.29 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 3 | 0.29 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 15 | 0.29 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 15 | 0.29 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 15 | 0.29 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 15 | 0.29 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 3 | 0.29 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 3 | 0.29 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 4 | 0.29 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 4 | 0.29 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 10 | 0.29 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 10 | 0.29 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 10 | 0.29 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 10 | 0.29 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 10 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 10 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 4 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 4 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 4 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 4 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 15 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 15 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 15 | 0.29 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 15 | 0.29 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 17 | 0.29 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 18 | 0.29 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 10 | 0.29 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 10 | 0.29 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 9 | 0.29 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 9 | 0.29 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 9 | 0.29 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 9 | 0.29 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 9 | 0.29 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 9 | 0.29 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 9 | 0.29 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 4 | 0.29 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 4 | 0.29 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 8 | 0.29 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 12 | 0.29 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 10 | 0.29 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 10 | 0.29 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 10 | 0.29 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 10 | 0.29 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 10 | 0.29 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 10 | 0.29 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 4 | 0.29 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 4 | 0.29 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 4 | 0.29 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 4 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 9 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 9 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 9 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 9 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 16 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 16 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 16 | 0.29 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 16 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 4 | 0.29 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 9 | 0.29 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 14 | 0.29 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 17 | 0.29 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 17 | 0.29 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 17 | 0.29 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 17 | 0.29 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 17 | 0.29 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 17 | 0.29 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 17 | 0.29 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 3 | 0.29 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 16 | 0.29 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 18 | 0.29 |
| (2,457) | 1:31:A:SER:H | 1:26:A:PHE:HD1 | 14 | 0.28 |
| (2,457) | 1:31:A:SER:H | 1:26:A:PHE:HD1 | 14 | 0.28 |
| (2,457) | 1:31:A:SER:H | 1:26:A:PHE:HD2 | 14 | 0.28 |
| (2,457) | 1:31:A:SER:H | 1:26:A:PHE:HD2 | 14 | 0.28 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 3 | 0.28 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 20 | 0.28 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 20 | 0.28 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 10 | 0.28 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 12 | 0.28 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 11 | 0.28 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 11 | 0.28 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 11 | 0.28 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 11 | 0.28 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 19 | 0.28 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 19 | 0.28 |
| (2,309) | 1:60:A:GLU:H | 1:61:A:PRO:HD2 | 19 | 0.28 |
| (2,309) | 1:60:A:GLU:H | 1:61:A:PRO:HD3 | 19 | 0.28 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 16 | 0.28 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 16 | 0.28 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 16 | 0.28 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 16 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 15 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 15 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 15 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 15 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 20 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD1 | 20 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 20 | 0.28 |
| (2,230) | 1:35:A:GLY:H | 1:34:A:PHE:HD2 | 20 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 2 | 0.28 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 2 | 0.28 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 2 | 0.28 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 2 | 0.28 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 12 | 0.28 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 12 | 0.28 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 12 | 0.28 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 12 | 0.28 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 12 | 0.28 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 12 | 0.28 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 12 | 0.28 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 12 | 0.28 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 16 | 0.28 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 11 | 0.28 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 11 | 0.28 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 11 | 0.28 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 11 | 0.28 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 11 | 0.28 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 11 | 0.28 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 3 | 0.28 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 14 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 2 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 2 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 2 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 2 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 10 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 10 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 10 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 10 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 11 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 11 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 11 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 11 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 13 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 13 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 13 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 13 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 17 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 17 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 17 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 17 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 20 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 20 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 20 | 0.28 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 20 | 0.28 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 1 | 0.28 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 2 | 0.28 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 3 | 0.28 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 12 | 0.28 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 18 | 0.28 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 5 | 0.28 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG2 | 5 | 0.28 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 5 | 0.28 |
| (2,25) | 1:22:A:ARG:H | 1:22:A:ARG:HG3 | 5 | 0.28 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 16 | 0.28 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 16 | 0.28 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 16 | 0.28 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 16 | 0.28 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 2 | 0.28 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 2 | 0.28 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 2 | 0.28 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 2 | 0.28 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 2 | 0.28 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 2 | 0.28 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 14 | 0.28 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 15 | 0.28 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 4 | 0.27 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 18 | 0.27 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 12 | 0.27 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 14 | 0.27 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 3 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 12 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 12 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 12 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 12 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 17 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 17 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 17 | 0.27 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 17 | 0.27 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 13 | 0.27 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 13 | 0.27 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 12 | 0.27 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 12 | 0.27 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 12 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 12 | 0.27 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 14 | 0.27 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG11 | 14 | 0.27 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 14 | 0.27 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG12 | 14 | 0.27 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 14 | 0.27 |
| (2,293) | 1:57:A:LEU:H | 1:56:A:VAL:HG13 | 14 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 5 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 5 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 5 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 5 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 12 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 12 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 12 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 12 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 17 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 17 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 17 | 0.27 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 17 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 13 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 13 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 13 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 13 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 13 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 13 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 15 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 15 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 15 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 15 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 15 | 0.27 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 15 | 0.27 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 19 | 0.27 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 19 | 0.27 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 19 | 0.27 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 19 | 0.27 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 19 | 0.27 |
| (2,201) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 19 | 0.27 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 12 | 0.27 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG2 | 19 | 0.27 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG3 | 19 | 0.27 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 14 | 0.27 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 14 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 14 | 0.27 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 14 | 0.27 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 8 | 0.27 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 20 | 0.27 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 5 | 0.27 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 6 | 0.27 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 4 | 0.27 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 1 | 0.27 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 9 | 0.27 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 11 | 0.27 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 16 | 0.26 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 3 | 0.26 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 9 | 0.26 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 9 | 0.26 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 9 | 0.26 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 9 | 0.26 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 9 | 0.26 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 9 | 0.26 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 2 | 0.26 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 20 | 0.26 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD21 | 20 | 0.26 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 20 | 0.26 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD22 | 20 | 0.26 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 20 | 0.26 |
| (2,322) | 1:63:A:ASN:H | 1:62:A:LEU:HD23 | 20 | 0.26 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 11 | 0.26 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 11 | 0.26 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 6 | 0.26 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 6 | 0.26 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 6 | 0.26 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 6 | 0.26 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 6 | 0.26 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 6 | 0.26 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 12 | 0.26 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 12 | 0.26 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 12 | 0.26 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 12 | 0.26 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 17 | 0.26 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 17 | 0.26 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 17 | 0.26 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 17 | 0.26 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 2 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 2 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 2 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 2 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 3 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 3 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 3 | 0.26 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 3 | 0.26 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 4 | 0.26 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 8 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 4 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 4 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 4 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 4 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 4 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 4 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 17 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 17 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 17 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 17 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 17 | 0.26 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 17 | 0.26 |
| (2,129) | 1:16:A:ALA:H | 1:15:A:THR:HG21 | 8 | 0.26 |
| (2,129) | 1:16:A:ALA:H | 1:15:A:THR:HG21 | 8 | 0.26 |
| (2,129) | 1:16:A:ALA:H | 1:15:A:THR:HG22 | 8 | 0.26 |
| (2,129) | 1:16:A:ALA:H | 1:15:A:THR:HG22 | 8 | 0.26 |
| (2,129) | 1:16:A:ALA:H | 1:15:A:THR:HG23 | 8 | 0.26 |
| (2,129) | 1:16:A:ALA:H | 1:15:A:THR:HG23 | 8 | 0.26 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 2 | 0.26 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 15 | 0.26 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD2 | 15 | 0.26 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 15 | 0.26 |
| (2,77) | 1:51:A:ARG:H | 1:51:A:ARG:HD3 | 15 | 0.26 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 5 | 0.26 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 6 | 0.26 |
| (2,44) | 1:28:A:VAL:H | 1:28:A:VAL:HB | 16 | 0.26 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 10 | 0.26 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 15 | 0.26 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 19 | 0.26 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 1 | 0.26 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 10 | 0.26 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 13 | 0.26 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 19 | 0.26 |
| (2,385) | 1:32:A:ASN:H | 1:30:A:SER:HA | 19 | 0.25 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 15 | 0.25 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 15 | 0.25 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 15 | 0.25 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 15 | 0.25 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 6 | 0.25 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 6 | 0.25 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 6 | 0.25 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 6 | 0.25 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 6 | 0.25 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 6 | 0.25 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 10 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 1 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 1 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 1 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 1 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 1 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 1 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 4 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 4 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 4 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 4 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 4 | 0.25 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 4 | 0.25 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 2 | 0.25 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 2 | 0.25 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 2 | 0.25 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 2 | 0.25 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 20 | 0.25 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 20 | 0.25 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 20 | 0.25 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 20 | 0.25 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 1 | 0.25 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 3 | 0.25 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 5 | 0.25 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 7 | 0.25 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 17 | 0.25 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 18 | 0.25 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 17 | 0.25 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 17 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 12 | 0.25 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 2 | 0.25 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 2 | 0.25 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 2 | 0.25 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 2 | 0.25 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 2 | 0.25 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 2 | 0.25 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 2 | 0.25 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 17 | 0.25 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 6 | 0.25 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 2 | 0.25 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 18 | 0.25 |
| (1,7) | 1:26:A:PHE:H | 1:22:A:ARG:O | 8 | 0.25 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 9 | 0.25 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 1 | 0.25 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 18 | 0.25 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 4 | 0.25 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 5 | 0.25 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 14 | 0.25 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 15 | 0.25 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 19 | 0.25 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 2 | 0.25 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 4 | 0.25 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 10 | 0.25 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 13 | 0.25 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 14 | 0.25 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 20 | 0.25 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 7 | 0.24 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 7 | 0.24 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 2 | 0.24 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 2 | 0.24 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 18 | 0.24 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 1 | 0.24 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 17 | 0.24 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 2 | 0.24 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 2 | 0.24 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 2 | 0.24 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 2 | 0.24 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 8 | 0.24 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 8 | 0.24 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 15 | 0.24 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 15 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 4 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 4 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 4 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 4 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 13 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 13 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 13 | 0.24 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 13 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 3 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 7 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 9 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 13 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 14 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 15 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 16 | 0.24 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 18 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 17 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 17 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 17 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 17 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 17 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 17 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 19 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 19 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 19 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 19 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 19 | 0.24 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 19 | 0.24 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 4 | 0.24 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 15 | 0.24 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 2 | 0.24 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 6 | 0.24 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 9 | 0.24 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 12 | 0.24 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 20 | 0.24 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 13 | 0.24 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 13 | 0.24 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 5 | 0.24 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 5 | 0.24 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 19 | 0.24 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB2 | 19 | 0.24 |
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 19 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,118) | 1:13:A:CYS:H | 1:12:A:LYS:HB3 | 19 | 0.24 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 3 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 7 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 7 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 7 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 7 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 9 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 9 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 9 | 0.24 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 9 | 0.24 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 7 | 0.24 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 9 | 0.24 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 14 | 0.24 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 1 | 0.24 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 4 | 0.24 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 19 | 0.24 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 19 | 0.24 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 7 | 0.24 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 11 | 0.24 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 12 | 0.24 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 7 | 0.24 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 12 | 0.24 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 17 | 0.24 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 1 | 0.24 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 5 | 0.24 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 11 | 0.23 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 13 | 0.23 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 7 | 0.23 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 3 | 0.23 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 3 | 0.23 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 3 | 0.23 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 3 | 0.23 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 9 | 0.23 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 9 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 1 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 1 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 1 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 1 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 2 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 2 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 2 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 2 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 5 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 5 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 5 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 5 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 6 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 6 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 6 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 6 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 10 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 10 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 10 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 10 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 11 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 11 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 11 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 11 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 12 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 12 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 12 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 12 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 15 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 15 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 15 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 15 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 16 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 16 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 16 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 16 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 18 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 18 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 18 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 18 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 20 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 20 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 20 | 0.23 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 20 | 0.23 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 2 | 0.23 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 11 | 0.23 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 12 | 0.23 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 17 | 0.23 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 19 | 0.23 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 20 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 5 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 5 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 5 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 5 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 5 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 5 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 8 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 8 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 8 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 8 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 8 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 8 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 18 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 18 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 18 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 18 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 18 | 0.23 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 18 | 0.23 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 13 | 0.23 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 2 | 0.23 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 6 | 0.23 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 18 | 0.23 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 8 | 0.23 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 8 | 0.23 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 4 | 0.23 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 10 | 0.23 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 1 | 0.23 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 17 | 0.23 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 17 | 0.23 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 17 | 0.23 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 17 | 0.23 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 16 | 0.23 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 16 | 0.23 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 16 | 0.23 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 16 | 0.23 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 2 | 0.23 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 11 | 0.23 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 13 | 0.23 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 17 | 0.23 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 15 | 0.23 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 5 | 0.23 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 11 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 16 | 0.23 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 13 | 0.23 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 14 | 0.23 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 19 | 0.23 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 20 | 0.23 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 4 | 0.23 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 5 | 0.23 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 6 | 0.23 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 6 | 0.23 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 7 | 0.23 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 18 | 0.23 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 5 | 0.22 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 4 | 0.22 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 17 | 0.22 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 11 | 0.22 |
| (2,333) | 1:15:A:THR:H | 1:18:A:CYS:H | 18 | 0.22 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 7 | 0.22 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 7 | 0.22 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 7 | 0.22 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 7 | 0.22 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 7 | 0.22 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 7 | 0.22 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 14 | 0.22 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 14 | 0.22 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 19 | 0.22 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 19 | 0.22 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 19 | 0.22 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 19 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 3 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 3 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 3 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 3 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 17 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 17 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 17 | 0.22 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 17 | 0.22 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 4 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 7 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 7 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 7 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 7 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 14 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 14 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 14 | 0.22 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 14 | 0.22 |
| (2,207) | 1:30:A:SER:H | 1:29:A:HIS:HA | 14 | 0.22 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 15 | 0.22 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 15 | 0.22 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 19 | 0.22 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 19 | 0.22 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 11 | 0.22 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 11 | 0.22 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 11 | 0.22 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 11 | 0.22 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 11 | 0.22 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 11 | 0.22 |
| (2,160) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 17 | 0.22 |
| (2,160) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 17 | 0.22 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 6 | 0.22 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 8 | 0.22 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 1 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 2 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 2 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 2 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 2 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 12 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 12 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 12 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 12 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 20 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 20 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 20 | 0.22 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 20 | 0.22 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 12 | 0.22 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 12 | 0.22 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 12 | 0.22 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 12 | 0.22 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 12 | 0.22 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 12 | 0.22 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 5 | 0.22 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 5 | 0.22 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 5 | 0.22 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 5 | 0.22 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 8 | 0.22 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 16 | 0.22 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 2 | 0.22 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 3 | 0.22 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 15 | 0.22 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 18 | 0.22 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 20 | 0.22 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 11 | 0.22 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 13 | 0.22 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 5 | 0.22 |
| (1,7) | 1:26:A:PHE:H | 1:22:A:ARG:O | 6 | 0.22 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 4 | 0.22 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 6 | 0.22 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 8 | 0.22 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 15 | 0.22 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 17 | 0.22 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 19 | 0.22 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 9 | 0.22 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 10 | 0.22 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 20 | 0.22 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 3 | 0.22 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 1 | 0.22 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 12 | 0.21 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 18 | 0.21 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 4 | 0.21 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 1 | 0.21 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 20 | 0.21 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 14 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 8 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 8 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 8 | 0.21 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 8 | 0.21 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 5 | 0.21 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 5 | 0.21 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 17 | 0.21 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 17 | 0.21 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 7 | 0.21 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 7 | 0.21 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 7 | 0.21 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 7 | 0.21 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 7 | 0.21 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 7 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 7 | 0.21 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 7 | 0.21 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 12 | 0.21 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 12 | 0.21 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 12 | 0.21 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 12 | 0.21 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 12 | 0.21 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 12 | 0.21 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 2 | 0.21 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 11 | 0.21 |
| (2,217) | 1:32:A:ASN:H | 1:31:A:SER:HA | 19 | 0.21 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 16 | 0.21 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 16 | 0.21 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 16 | 0.21 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 16 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 1 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 1 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 1 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 1 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 9 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 9 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 9 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 9 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 17 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 17 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 17 | 0.21 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 17 | 0.21 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 11 | 0.21 |
| (2,205) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 11 | 0.21 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG11 | 19 | 0.21 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG12 | 19 | 0.21 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG13 | 19 | 0.21 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG21 | 19 | 0.21 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG22 | 19 | 0.21 |
| (2,202) | 1:29:A:HIS:H | 1:28:A:VAL:HG23 | 19 | 0.21 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 16 | 0.21 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 16 | 0.21 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 8 | 0.21 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 13 | 0.21 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 13 | 0.21 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 2 | 0.21 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 9 | 0.21 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 9 | 0.21 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 17 | 0.21 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 17 | 0.21 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 10 | 0.21 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 8 | 0.21 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 14 | 0.21 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 12 | 0.21 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 16 | 0.21 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 5 | 0.21 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 13 | 0.21 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 18 | 0.21 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 10 | 0.21 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 13 | 0.21 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 15 | 0.21 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 1 | 0.21 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 18 | 0.21 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 1 | 0.21 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 2 | 0.21 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 3 | 0.21 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 18 | 0.21 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 13 | 0.21 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 8 | 0.21 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 7 | 0.21 |
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 12 | 0.21 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 4 | 0.21 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 14 | 0.21 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 19 | 0.21 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 6 | 0.2 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 14 | 0.2 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 20 | 0.2 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 20 | 0.2 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 20 | 0.2 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 20 | 0.2 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD2 | 10 | 0.2 |
| (2,313) | 1:62:A:LEU:H | 1:61:A:PRO:HD3 | 10 | 0.2 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 1 | 0.2 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 1 | 0.2 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 1 | 0.2 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 1 | 0.2 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 1 | 0.2 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 12 | 0.2 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 1 | 0.2 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 11 | 0.2 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 11 | 0.2 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 6 | 0.2 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 6 | 0.2 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 10 | 0.2 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 13 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 1 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 1 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 1 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 1 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 6 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 6 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 6 | 0.2 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 6 | 0.2 |
| (1,20) | 1:65:A:LEU:H | 1:61:A:PRO:O | 3 | 0.2 |
| (1,18) | 1:59:A:ARG:H | 1:55:A:GLU:O | 15 | 0.2 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 1 | 0.2 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 4 | 0.2 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 20 | 0.2 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 2 | 0.2 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 5 | 0.2 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 11 | 0.2 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 8 | 0.2 |
| (1,7) | 1:26:A:PHE:H | 1:22:A:ARG:O | 5 | 0.2 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 11 | 0.2 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 15 | 0.2 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 2 | 0.2 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 11 | 0.2 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 12 | 0.2 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 18 | 0.2 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 19 | 0.2 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 8 | 0.19 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 8 | 0.19 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 8 | 0.19 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 8 | 0.19 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 7 | 0.19 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 9 | 0.19 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 14 | 0.19 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 9 | 0.19 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 9 | 0.19 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 9 | 0.19 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 9 | 0.19 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 9 | 0.19 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 2 | 0.19 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 17 | 0.19 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 8 | 0.19 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 12 | 0.19 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 20 | 0.19 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 20 | 0.19 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 20 | 0.19 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 20 | 0.19 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 20 | 0.19 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 18 | 0.19 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB2 | 18 | 0.19 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 18 | 0.19 |
| (2,214) | 1:32:A:ASN:H | 1:31:A:SER:HB3 | 18 | 0.19 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 6 | 0.19 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 6 | 0.19 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 20 | 0.19 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 15 | 0.19 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 15 | 0.19 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 5 | 0.19 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 5 | 0.19 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 7 | 0.19 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 7 | 0.19 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 20 | 0.19 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 20 | 0.19 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 6 | 0.19 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 6 | 0.19 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 5 | 0.19 |
| (2,128) | 1:15:A:THR:H | 1:14:A:ASN:HB2 | 2 | 0.19 |
| (2,128) | 1:15:A:THR:H | 1:14:A:ASN:HB3 | 2 | 0.19 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 9 | 0.19 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 3 | 0.19 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 6 | 0.19 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 10 | 0.19 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 20 | 0.19 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 5 | 0.19 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 20 | 0.19 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 16 | 0.19 |
| (1,4) | 1:23:A:LEU:H | 1:19:A:ALA:O | 17 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,3) | 1:22:A:ARG:H | 1:18:A:CYS:O | 18 | 0.19 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 16 | 0.19 |
| (2,400) | 1:36:A:ALA:H | 1:34:A:PHE:HA | 9 | 0.18 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 1 | 0.18 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 8 | 0.18 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 19 | 0.18 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 20 | 0.18 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 10 | 0.18 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 13 | 0.18 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 19 | 0.18 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 10 | 0.18 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 14 | 0.18 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 14 | 0.18 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 14 | 0.18 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 14 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 5 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 5 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 5 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 5 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 13 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 13 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 13 | 0.18 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 13 | 0.18 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 8 | 0.18 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 3 | 0.18 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 11 | 0.18 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 13 | 0.18 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 15 | 0.18 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 16 | 0.18 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 16 | 0.18 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 16 | 0.18 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 16 | 0.18 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 16 | 0.18 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 16 | 0.18 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 8 | 0.18 |
| (2,232) | 1:36:A:ALA:H | 1:37:A:ILE:HG12 | 14 | 0.18 |
| (2,232) | 1:36:A:ALA:H | 1:37:A:ILE:HG13 | 14 | 0.18 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 17 | 0.18 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB2 | 17 | 0.18 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 17 | 0.18 |
| (2,223) | 1:34:A:PHE:H | 1:33:A:ASN:HB3 | 17 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 1 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 1 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 1 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 1 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 8 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 8 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 8 | 0.18 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 8 | 0.18 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 10 | 0.18 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 10 | 0.18 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 10 | 0.18 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 10 | 0.18 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 12 | 0.18 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 12 | 0.18 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 8 | 0.18 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 14 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 7 | 0.18 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 7 | 0.18 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 3 | 0.18 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 8 | 0.18 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB2 | 8 | 0.18 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 8 | 0.18 |
| (2,13) | 1:18:A:CYS:H | 1:18:A:CYS:HB3 | 8 | 0.18 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 20 | 0.18 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 20 | 0.18 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 20 | 0.18 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 20 | 0.18 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 20 | 0.18 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 20 | 0.18 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 17 | 0.18 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 17 | 0.18 |
| (1,18) | 1:59:A:ARG:H | 1:55:A:GLU:O | 14 | 0.18 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 3 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 9 | 0.18 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 16 | 0.18 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 6 | 0.18 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 10 | 0.17 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 8 | 0.17 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 18 | 0.17 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 5 | 0.17 |
| (2,273) | 1:53:A:ALA:H | 1:52:A:ASN:HA | 6 | 0.17 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 2 | 0.17 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 20 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 2 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 2 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 2 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 2 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 2 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 2 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 20 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 20 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 20 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 20 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 20 | 0.17 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 20 | 0.17 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 6 | 0.17 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 16 | 0.17 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 16 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 18 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 18 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 18 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 18 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 20 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 20 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 20 | 0.17 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 20 | 0.17 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 19 | 0.17 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 19 | 0.17 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 4 | 0.17 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 4 | 0.17 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 15 | 0.17 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 15 | 0.17 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 10 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 7 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 7 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 7 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 10 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 10 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 10 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 10 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 14 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 14 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 14 | 0.17 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 14 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 2 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 13 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 18 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 18 | 0.17 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 18 | 0.17 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 16 | 0.17 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 14 | 0.17 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 14 | 0.17 |
| (1,17) | 1:58:A:LYS:H | 1:54:A:VAL:O | 8 | 0.17 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 18 | 0.17 |
| (1,6) | 1:25:A:ASN:H | 1:21:A:GLN:O | 5 | 0.17 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 13 | 0.16 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD21 | 8 | 0.16 |
| (2,419) | 1:54:A:VAL:H | 1:52:A:ASN:HD22 | 8 | 0.16 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 6 | 0.16 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 16 | 0.16 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 2 | 0.16 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 15 | 0.16 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 14 | 0.16 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 15 | 0.16 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 12 | 0.16 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 16 | 0.16 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 17 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 13 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 13 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 13 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 13 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 13 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 13 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 15 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 15 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 15 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 15 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 15 | 0.16 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 15 | 0.16 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 3 | 0.16 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 5 | 0.16 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 7 | 0.16 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 18 | 0.16 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 20 | 0.16 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 3 | 0.16 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 6 | 0.16 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 6 | 0.16 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 6 | 0.16 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 6 | 0.16 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 10 | 0.16 |
| (2,192) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 10 | 0.16 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 3 | 0.16 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 3 | 0.16 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 13 | 0.16 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 13 | 0.16 |
| (2,160) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 6 | 0.16 |
| (2,160) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 6 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 9 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 9 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 9 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 9 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 11 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 11 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 11 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 11 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 13 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 13 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 13 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 13 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 20 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 20 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 20 | 0.16 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 20 | 0.16 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 10 | 0.16 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 14 | 0.16 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 8 | 0.16 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG21 | 8 | 0.16 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 8 | 0.16 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG22 | 8 | 0.16 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 8 | 0.16 |
| (2,6) | 1:15:A:THR:H | 1:15:A:THR:HG23 | 8 | 0.16 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 2 | 0.16 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 2 | 0.16 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 6 | 0.16 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 16 | 0.16 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 9 | 0.16 |
| (1,5) | 1:24:A:ALA:H | 1:20:A:THR:O | 16 | 0.16 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 20 | 0.16 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 5 | 0.16 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 20 | 0.15 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 9 | 0.15 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 14 | 0.15 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG21 | 14 | 0.15 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 14 | 0.15 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG22 | 14 | 0.15 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 14 | 0.15 |
| (2,336) | 1:17:A:THR:H | 1:15:A:THR:HG23 | 14 | 0.15 |
| (2,333) | 1:15:A:THR:H | 1:18:A:CYS:H | 11 | 0.15 |
| (2,333) | 1:15:A:THR:H | 1:18:A:CYS:H | 13 | 0.15 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 1 | 0.15 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 1 | 0.15 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 1 | 0.15 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 1 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 8 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 8 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 8 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 8 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 9 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG2 | 9 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 9 | 0.15 |
| (2,292) | 1:56:A:VAL:H | 1:55:A:GLU:HG3 | 9 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 7 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 7 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 7 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 7 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 10 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 10 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 10 | 0.15 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 10 | 0.15 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 1 | 0.15 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 4 | 0.15 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 5 | 0.15 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 18 | 0.15 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 19 | 0.15 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 10 | 0.15 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 10 | 0.15 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 10 | 0.15 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 10 | 0.15 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 10 | 0.15 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 10 | 0.15 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 13 | 0.15 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 5 | 0.15 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 3 | 0.15 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 3 | 0.15 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 3 | 0.15 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 3 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 3 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 3 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 3 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 3 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 3 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 4 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 4 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 4 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 4 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 5 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 5 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 5 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 5 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 7 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 7 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 7 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 7 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 11 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 11 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 11 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 11 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 19 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 19 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 19 | 0.15 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 19 | 0.15 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 20 | 0.15 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 20 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 1 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 1 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 14 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 14 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 16 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 16 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 19 | 0.15 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,146) | 1:19:A:ALA:H | 1:20:A:THR:HA | 8 | 0.15 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 1 | 0.15 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 15 | 0.15 |
| (2,131) | 1:16:A:ALA:H | 1:17:A:THR:H | 2 | 0.15 |
| (2,131) | 1:16:A:ALA:H | 1:17:A:THR:H | 17 | 0.15 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 9 | 0.15 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 20 | 0.15 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG21 | 20 | 0.15 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 20 | 0.15 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG22 | 20 | 0.15 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 20 | 0.15 |
| (2,121) | 1:14:A:ASN:H | 1:15:A:THR:HG23 | 20 | 0.15 |
| (2,114) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 20 | 0.15 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 17 | 0.15 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 17 | 0.15 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 17 | 0.15 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 17 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 12 | 0.15 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 12 | 0.15 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 9 | 0.15 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 10 | 0.15 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 10 | 0.15 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 12 | 0.15 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 12 | 0.15 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 4 | 0.15 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 18 | 0.14 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 19 | 0.14 |
| (2,385) | 1:32:A:ASN:H | 1:30:A:SER:HA | 11 | 0.14 |
| (2,369) | 1:28:A:VAL:H | 1:29:A:HIS:H | 5 | 0.14 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 4 | 0.14 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB2 | 4 | 0.14 |
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,332) | 1:15:A:THR:H | 1:18:A:CYS:HB3 | 4 | 0.14 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 5 | 0.14 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 16 | 0.14 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 16 | 0.14 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 16 | 0.14 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 16 | 0.14 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 2 | 0.14 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 3 | 0.14 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 11 | 0.14 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 18 | 0.14 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 10 | 0.14 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 10 | 0.14 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 6 | 0.14 |
| (2,265) | 1:52:A:ASN:H | 1:51:A:ARG:HA | 8 | 0.14 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 4 | 0.14 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 11 | 0.14 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 18 | 0.14 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 8 | 0.14 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 8 | 0.14 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 8 | 0.14 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 8 | 0.14 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 10 | 0.14 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 10 | 0.14 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 10 | 0.14 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 10 | 0.14 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 1 | 0.14 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 1 | 0.14 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 8 | 0.14 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 8 | 0.14 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 11 | 0.14 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 11 | 0.14 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB2 | 18 | 0.14 |
| (2,167) | 1:23:A:LEU:H | 1:22:A:ARG:HB3 | 18 | 0.14 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 19 | 0.14 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 14 | 0.14 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 7 | 0.14 |
| (2,109) | 1:60:A:GLU:H | 1:60:A:GLU:HG2 | 19 | 0.14 |
| (2,109) | 1:60:A:GLU:H | 1:60:A:GLU:HG3 | 19 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 1 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 1 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 1 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 8 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 8 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 8 | 0.14 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 8 | 0.14 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 2 | 0.14 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 4 | 0.14 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 12 | 0.14 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 10 | 0.14 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 16 | 0.14 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 4 | 0.13 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 11 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 1 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 1 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 1 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 1 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 10 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 10 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 10 | 0.13 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 10 | 0.13 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 1 | 0.13 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 4 | 0.13 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 5 | 0.13 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 9 | 0.13 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 12 | 0.13 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 20 | 0.13 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 14 | 0.13 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 14 | 0.13 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 14 | 0.13 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 14 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 3 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 3 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 3 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 3 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 3 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 3 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 7 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB1 | 7 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 7 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB2 | 7 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 7 | 0.13 |
| (2,260) | 1:51:A:ARG:H | 1:53:A:ALA:HB3 | 7 | 0.13 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 17 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 9 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 9 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 9 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 9 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 15 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 15 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 15 | 0.13 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 15 | 0.13 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 13 | 0.13 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 13 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 4 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 4 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 4 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 4 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 5 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 5 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 5 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 5 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 12 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 12 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 12 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 12 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 16 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 16 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 16 | 0.13 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 16 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 11 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 14 | 0.13 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 14 | 0.13 |
| (2,71) | 1:37:A:ILE:H | 1:37:A:ILE:HG12 | 8 | 0.13 |
| (2,71) | 1:37:A:ILE:H | 1:37:A:ILE:HG13 | 8 | 0.13 |
| (2,68) | 1:37:A:ILE:H | 1:37:A:ILE:HG12 | 14 | 0.13 |
| (2,68) | 1:37:A:ILE:H | 1:37:A:ILE:HG13 | 14 | 0.13 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 8 | 0.13 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 8 | 0.13 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 8 | 0.13 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 8 | 0.13 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 12 | 0.13 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 7 | 0.13 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 7 | 0.13 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 12 | 0.13 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 12 | 0.13 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 12 | 0.13 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 12 | 0.13 |
| (1,16) | 1:57:A:LEU:H | 1:53:A:ALA:O | 1 | 0.13 |
| (1,13) | 1:39:A:SER:H | 1:35:A:GLY:O | 2 | 0.13 |
| (1,8) | 1:27:A:LEU:H | 1:23:A:LEU:O | 6 | 0.13 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 9 | 0.13 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 4 | 0.13 |
| (2,451) | 1:65:A:LEU:H | 1:62:A:LEU:HA | 2 | 0.12 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 7 | 0.12 |
| (2,400) | 1:36:A:ALA:H | 1:34:A:PHE:HA | 7 | 0.12 |
| (2,385) | 1:32:A:ASN:H | 1:30:A:SER:HA | 15 | 0.12 |
| (2,373) | 1:30:A:SER:H | 1:26:A:PHE:HA | 10 | 0.12 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 19 | 0.12 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 9 | 0.12 |
| (2,328) | 1:14:A:ASN:H | 1:18:A:CYS:HB2 | 8 | 0.12 |
| (2,328) | 1:14:A:ASN:H | 1:18:A:CYS:HB2 | 8 | 0.12 |
| (2,328) | 1:14:A:ASN:H | 1:18:A:CYS:HB3 | 8 | 0.12 |
| (2,328) | 1:14:A:ASN:H | 1:18:A:CYS:HB3 | 8 | 0.12 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 4 | 0.12 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 4 | 0.12 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 4 | 0.12 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 14 | 0.12 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB2 | 14 | 0.12 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 14 | 0.12 |
| (2,285) | 1:56:A:VAL:H | 1:55:A:GLU:HB3 | 14 | 0.12 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 6 | 0.12 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 7 | 0.12 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 8 | 0.12 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 16 | 0.12 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 9 | 0.12 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB2 | 9 | 0.12 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 9 | 0.12 |
| (2,274) | 1:53:A:ALA:H | 1:52:A:ASN:HB3 | 9 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 9 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 9 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 15 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 15 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 20 | 0.12 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 20 | 0.12 |
| (2,255) | 1:39:A:SER:H | 1:38:A:LEU:HA | 9 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 2 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 2 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 2 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 2 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 8 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 8 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 8 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 8 | 0.12 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 8 | 0.12 |
| (2,252) | 1:38:A:LEU:H | 1:39:A:SER:HA | 4 | 0.12 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 2 | 0.12 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 2 | 0.12 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 2 | 0.12 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 2 | 0.12 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 2 | 0.12 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 2 | 0.12 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB2 | 18 | 0.12 |
| (2,199) | 1:28:A:VAL:H | 1:27:A:LEU:HB3 | 18 | 0.12 |
| (2,197) | 1:28:A:VAL:H | 1:27:A:LEU:HG | 16 | 0.12 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 16 | 0.12 |
| (2,123) | 1:14:A:ASN:H | 1:15:A:THR:H | 5 | 0.12 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG2 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG3 | 17 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 6 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 6 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 6 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 6 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 15 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 15 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 15 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 15 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 18 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 18 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 18 | 0.12 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 18 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 17 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 19 | 0.12 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 19 | 0.12 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 16 | 0.12 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 16 | 0.12 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 16 | 0.12 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 16 | 0.12 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 20 | 0.12 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 20 | 0.12 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 20 | 0.12 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 20 | 0.12 |
| (1,9) | 1:28:A:VAL:H | 1:24:A:ALA:O | 7 | 0.12 |
| (1,2) | 1:21:A:GLN:H | 1:17:A:THR:O | 17 | 0.12 |
| (2,450) | 1:64:A:TYR:H | 1:62:A:LEU:H | 8 | 0.11 |
| (2,429) | 1:57:A:LEU:H | 1:56:A:VAL:HB | 7 | 0.11 |
| (2,400) | 1:36:A:ALA:H | 1:34:A:PHE:HA | 15 | 0.11 |
| (2,367) | 1:28:A:VAL:H | 1:24:A:ALA:HA | 5 | 0.11 |
| (2,361) | 1:25:A:ASN:H | 1:23:A:LEU:HA | 4 | 0.11 |
| (2,329) | 1:14:A:ASN:H | 1:12:A:LYS:HA | 6 | 0.11 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 18 | 0.11 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 18 | 0.11 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 18 | 0.11 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 18 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 7 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 7 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 7 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 7 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 17 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 17 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 17 | 0.11 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 17 | 0.11 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 10 | 0.11 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 13 | 0.11 |
| (2,279) | 1:55:A:GLU:H | 1:54:A:VAL:HB | 19 | 0.11 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 7 | 0.11 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 7 | 0.11 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 13 | 0.11 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 13 | 0.11 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 12 | 0.11 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB2 | 12 | 0.11 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 12 | 0.11 |
| (2,254) | 1:39:A:SER:H | 1:38:A:LEU:HB3 | 12 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 10 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 10 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 10 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 10 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 18 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB2 | 18 | 0.11 |
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,219) | 1:33:A:ASN:H | 1:32:A:ASN:HB3 | 18 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 14 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 14 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 14 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 14 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 17 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 17 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 17 | 0.11 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 17 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 11 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 11 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 15 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 15 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB2 | 19 | 0.11 |
| (2,208) | 1:30:A:SER:H | 1:29:A:HIS:HB3 | 19 | 0.11 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB2 | 5 | 0.11 |
| (2,161) | 1:22:A:ARG:H | 1:21:A:GLN:HB3 | 5 | 0.11 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG2 | 2 | 0.11 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG3 | 2 | 0.11 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG2 | 12 | 0.11 |
| (2,106) | 1:60:A:GLU:H | 1:60:A:GLU:HG3 | 12 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 2 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 2 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 2 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 2 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 3 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 3 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 3 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 3 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 19 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB2 | 19 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 19 | 0.11 |
| (2,105) | 1:59:A:ARG:H | 1:59:A:ARG:HB3 | 19 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|--------------|-----------------|----------|---------------|
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 4 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD11 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD12 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD13 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD21 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD22 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 5 | 0.11 |
| (2,95) | 1:57:A:LEU:H | 1:57:A:LEU:HD23 | 5 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 4 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 4 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 4 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 4 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 9 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 9 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 9 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 9 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 10 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 10 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 10 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 10 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 11 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 11 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 11 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 11 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 12 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 12 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 12 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 12 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 15 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 15 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 15 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 15 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 18 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 18 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 18 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 20 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 20 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 20 | 0.11 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 20 | 0.11 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 7 | 0.11 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 13 | 0.11 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 15 | 0.11 |
| (2,4) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 15 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 3 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 3 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 3 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 3 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 7 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB2 | 7 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 7 | 0.11 |
| (2,2) | 1:13:A:CYS:H | 1:13:A:CYS:HB3 | 7 | 0.11 |
| (1,10) | 1:36:A:ALA:H | 1:32:A:ASN:O | 14 | 0.11 |
| (1,1) | 1:20:A:THR:H | 1:16:A:ALA:O | 11 | 0.11 |
| (2,386) | 1:32:A:ASN:H | 1:34:A:PHE:H | 16 | 0.1 |
| (2,373) | 1:30:A:SER:H | 1:26:A:PHE:HA | 19 | 0.1 |
| (2,321) | 1:63:A:ASN:H | 1:62:A:LEU:HA | 18 | 0.1 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 13 | 0.1 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG2 | 13 | 0.1 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 13 | 0.1 |
| (2,316) | 1:62:A:LEU:H | 1:61:A:PRO:HG3 | 13 | 0.1 |
| (2,315) | 1:62:A:LEU:H | 1:61:A:PRO:HA | 9 | 0.1 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 14 | 0.1 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB2 | 14 | 0.1 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 14 | 0.1 |
| (2,312) | 1:60:A:GLU:H | 1:59:A:ARG:HB3 | 14 | 0.1 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 12 | 0.1 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 12 | 0.1 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD21 | 18 | 0.1 |
| (2,270) | 1:53:A:ALA:H | 1:52:A:ASN:HD22 | 18 | 0.1 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 13 | 0.1 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB2 | 13 | 0.1 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 13 | 0.1 |
| (2,216) | 1:32:A:ASN:H | 1:33:A:ASN:HB3 | 13 | 0.1 |
| (2,190) | 1:27:A:LEU:H | 1:26:A:PHE:HB2 | 16 | 0.1 |
| (2,190) | 1:27:A:LEU:H | 1:26:A:PHE:HB3 | 16 | 0.1 |
| (2,139) | 1:18:A:CYS:H | 1:17:A:THR:HB | 11 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (2,131) | 1:16:A:ALA:H | 1:17:A:THR:H | 4 | 0.1 |
| (2,125) | 1:15:A:THR:H | 1:14:A:ASN:H | 7 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 1 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 1 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 1 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 1 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 2 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 2 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 2 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 2 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 3 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 3 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 3 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 3 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 7 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 7 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 7 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 7 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 17 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 17 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 17 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 17 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 19 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB2 | 19 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 19 | 0.1 |
| (2,58) | 1:33:A:ASN:H | 1:33:A:ASN:HB3 | 19 | 0.1 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 11 | 0.1 |
| (2,20) | 1:21:A:GLN:H | 1:21:A:GLN:HG3 | 18 | 0.1 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 14 | 0.1 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 14 | 0.1 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB2 | 17 | 0.1 |
| (2,5) | 1:14:A:ASN:H | 1:14:A:ASN:HB3 | 17 | 0.1 |

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

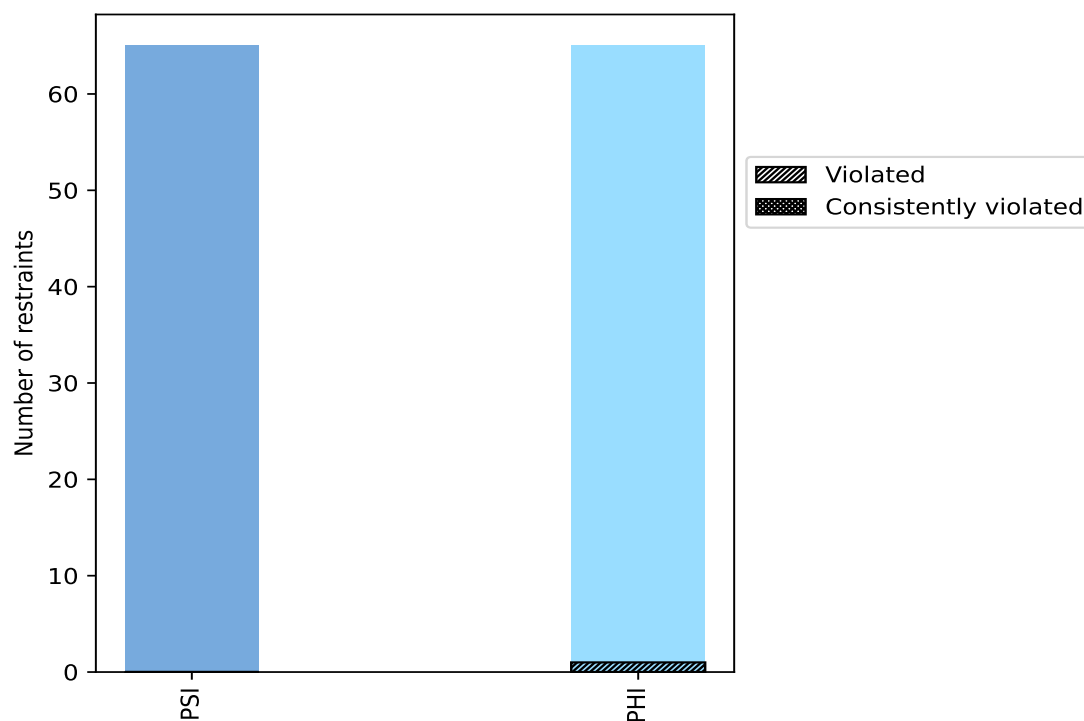
10.1 Summary of dihedral-angle violations [i](#)

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 | 65 | 50.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| PHI | 65 | 50.0 | 1 | 1.5 | 0.8 | 0 | 0.0 | 0.0 |
| Total | 130 | 100.0 | 1 | 0.8 | 0.8 | 0 | 0.0 | 0.0 |

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

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



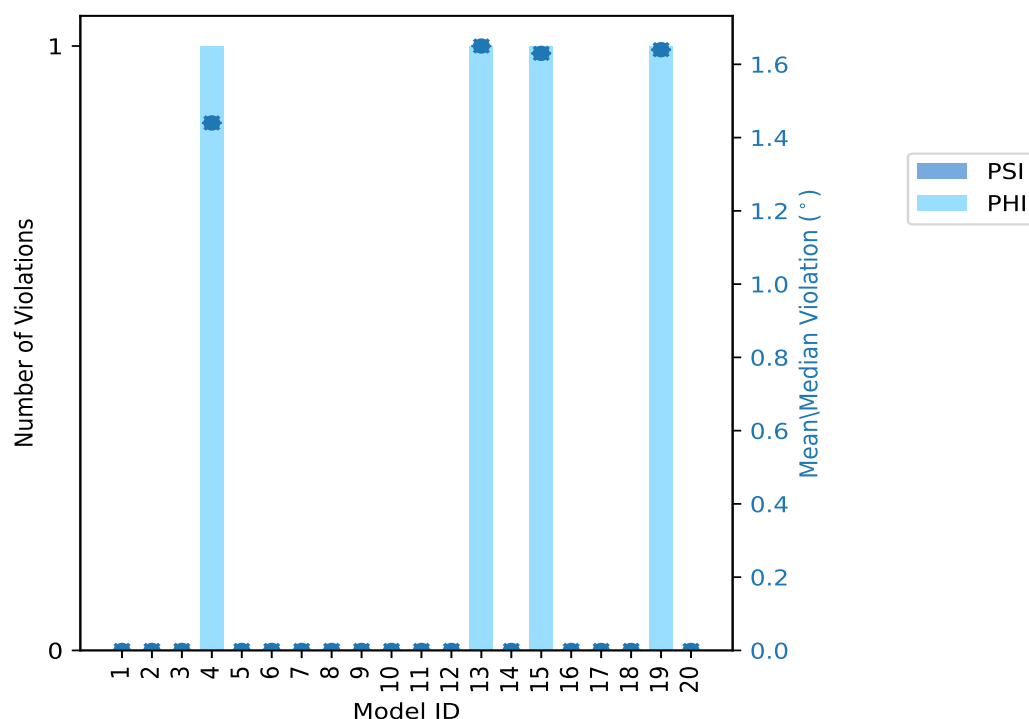
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 2 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 3 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 4 | 0 | 1 | 1 | 1.44 | 1.44 | 0.0 | 1.44 |
| 5 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 6 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 7 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 8 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 9 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 10 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 11 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 12 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13 | 0 | 1 | 1 | 1.65 | 1.65 | 0.0 | 1.65 |
| 14 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 | 0 | 1 | 1 | 1.63 | 1.63 | 0.0 | 1.63 |
| 16 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 17 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 18 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 19 | 0 | 1 | 1 | 1.64 | 1.64 | 0.0 | 1.64 |
| 20 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |

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

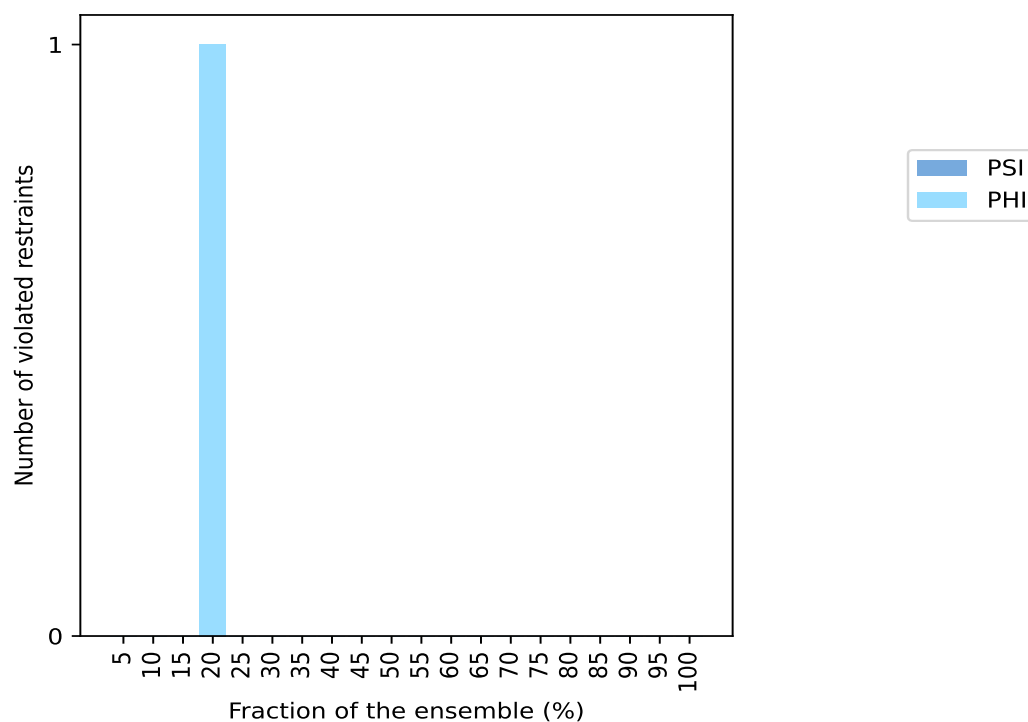
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 |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

¹ Number of models with violations

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

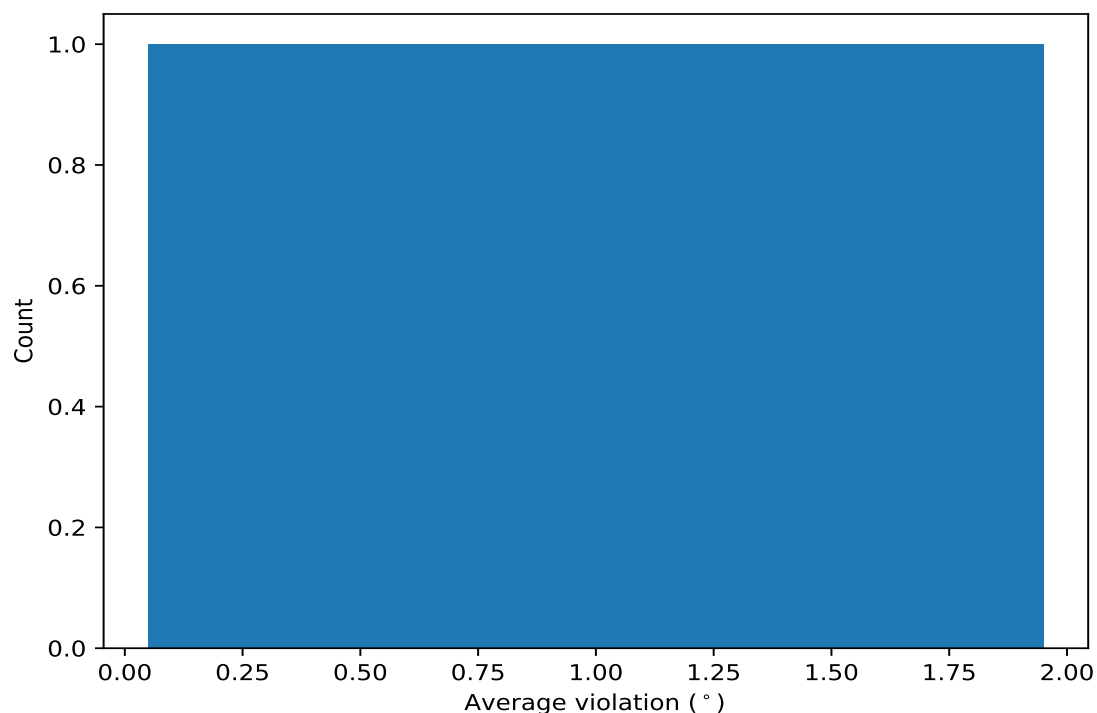


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|--------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,11) | 1:12:A:LYS:C | 1:13:A:CYS:N | 1:13:A:CYS:CA | 1:13:A:CYS:C | 4 | 1.59 | 0.09 | 1.63 |

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.

Data insufficient to plot histogram

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 (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,11) | 1:12:A:LYS:C | 1:13:A:CYS:N | 1:13:A:CYS:CA | 1:13:A:CYS:C | 13 | 1.65 |
| (1,11) | 1:12:A:LYS:C | 1:13:A:CYS:N | 1:13:A:CYS:CA | 1:13:A:CYS:C | 19 | 1.64 |
| (1,11) | 1:12:A:LYS:C | 1:13:A:CYS:N | 1:13:A:CYS:CA | 1:13:A:CYS:C | 15 | 1.63 |
| (1,11) | 1:12:A:LYS:C | 1:13:A:CYS:N | 1:13:A:CYS:CA | 1:13:A:CYS:C | 4 | 1.44 |