



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2024 – 12:09 PM JST

PDB ID : 8X8T
BMRB ID : 36619
Title : NMR structure of p75NTR juxtamembrane domain in complex with RhoGDI N-terminal domain containing a phosphorylation-mimicking S34D mutation
Authors : Lin, Z.; Li, Z.
Deposited on : 2023-11-28

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.36

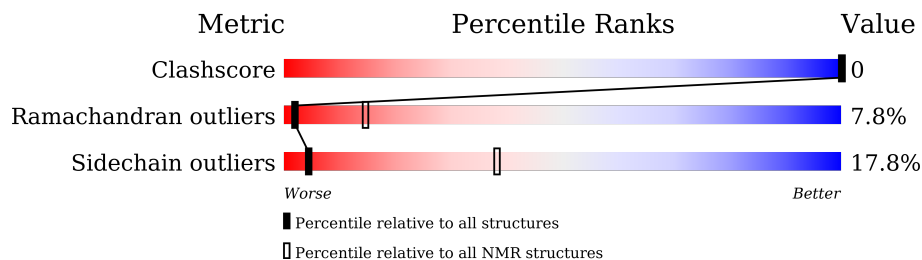
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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 | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

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 | 61 | 72% 13% 15% |
| 2 | B | 62 | 56% 10% 34% |

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:8-A:59, B:285-B:325 (93) | 1.20 | 2 |

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

| Cluster number | Models |
|-----------------------|-------------|
| 1 | 2, 3, 6, 10 |
| 2 | 4, 5, 8 |
| 3 | 1, 9 |
| Single-model clusters | 7 |

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1849 atoms, of which 899 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Rho GDP-dissociation inhibitor 1.

| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|-------|
| | | | Total | C | H | N | O | |
| 1 | A | 61 | 942 | 293 | 459 | 82 | 108 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 0 | GLY | - | expression tag | UNP P52565 |
| A | 1 | SER | - | expression tag | UNP P52565 |
| A | 34 | ASP | SER | engineered mutation | UNP P52565 |

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 16.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| | | | Total | C | H | N | O | S | |
| 2 | B | 62 | 907 | 275 | 440 | 92 | 99 | 1 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

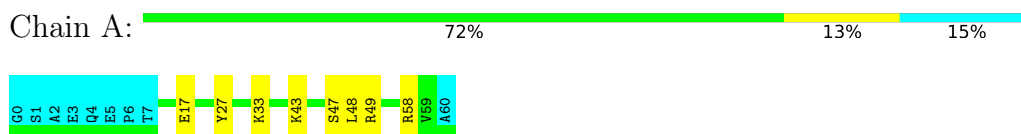
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 271 | GLY | - | expression tag | UNP P08138 |
| B | 272 | SER | - | expression tag | UNP P08138 |

4 Residue-property plots i

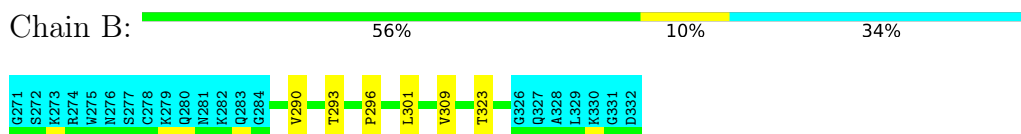
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Rho GDP-dissociation inhibitor 1



- Molecule 2: Tumor necrosis factor receptor superfamily member 16

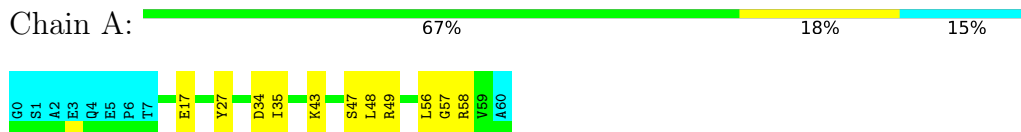


4.2 Scores per residue for each member of the ensemble

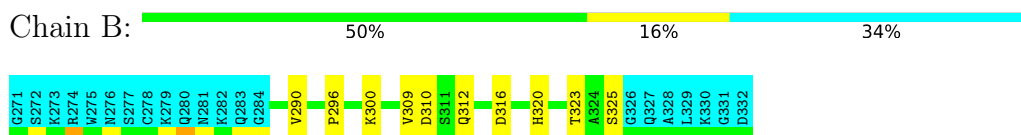
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Rho GDP-dissociation inhibitor 1

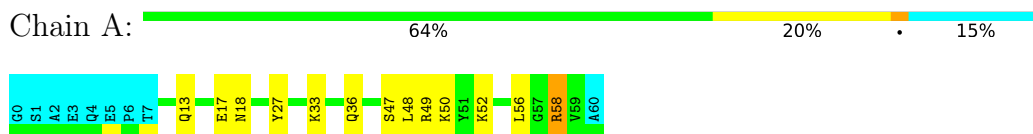


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

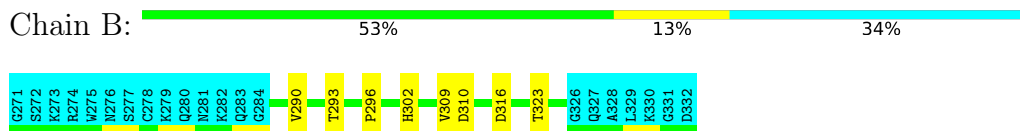


4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Rho GDP-dissociation inhibitor 1

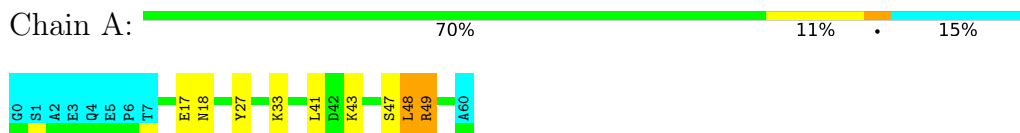


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

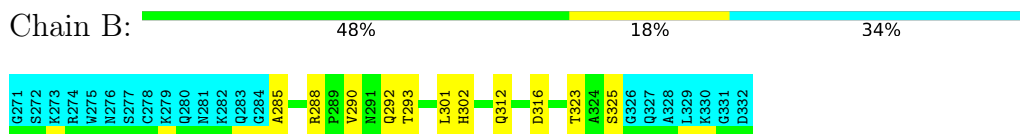


4.2.3 Score per residue for model 3

- Molecule 1: Rho GDP-dissociation inhibitor 1

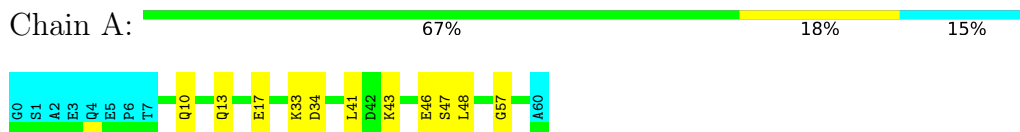


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

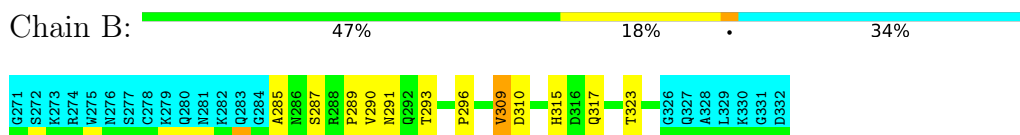


4.2.4 Score per residue for model 4

- Molecule 1: Rho GDP-dissociation inhibitor 1

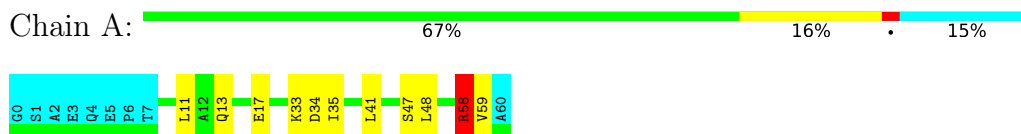


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

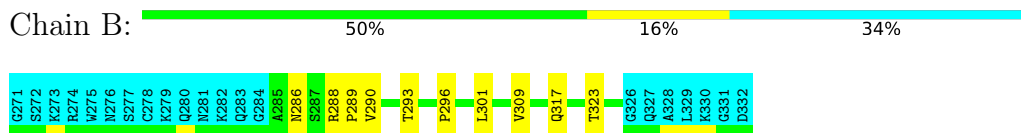


4.2.5 Score per residue for model 5

- Molecule 1: Rho GDP-dissociation inhibitor 1

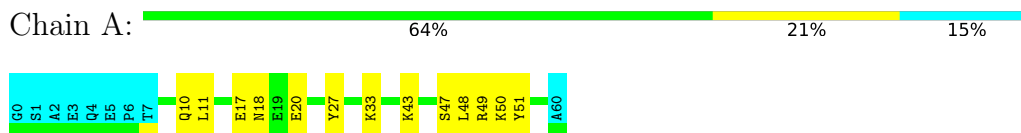


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

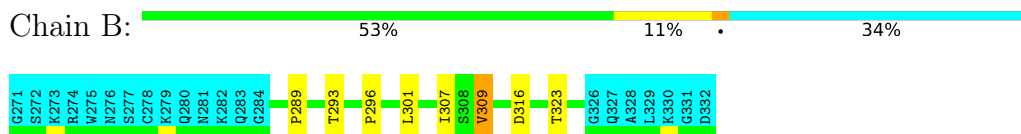


4.2.6 Score per residue for model 6

- Molecule 1: Rho GDP-dissociation inhibitor 1

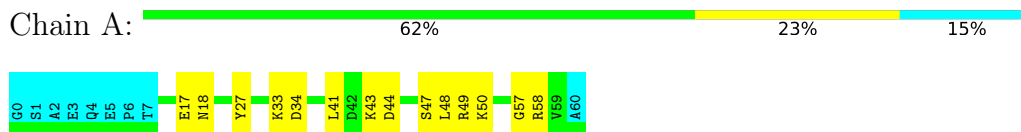


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

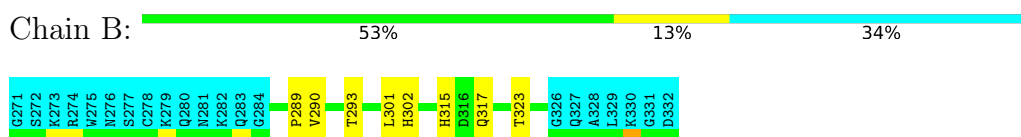


4.2.7 Score per residue for model 7

- Molecule 1: Rho GDP-dissociation inhibitor 1

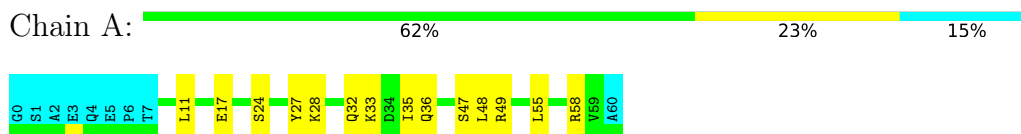


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

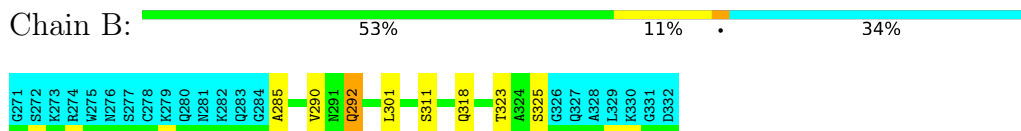


4.2.8 Score per residue for model 8

- Molecule 1: Rho GDP-dissociation inhibitor 1

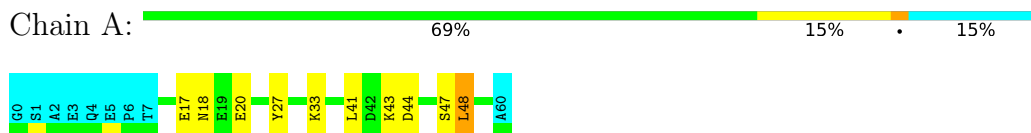


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

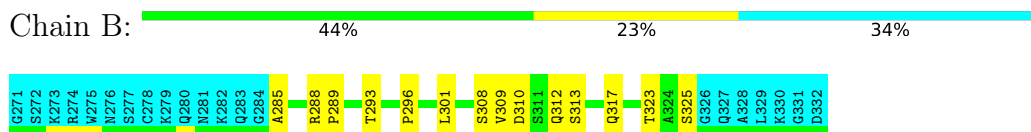


4.2.9 Score per residue for model 9

- Molecule 1: Rho GDP-dissociation inhibitor 1

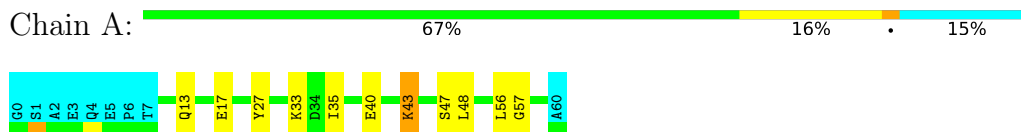


- Molecule 2: Tumor necrosis factor receptor superfamily member 16

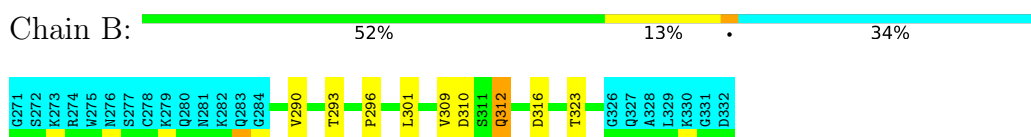


4.2.10 Score per residue for model 10

- Molecule 1: Rho GDP-dissociation inhibitor 1



- Molecule 2: Tumor necrosis factor receptor superfamily member 16



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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 |
|---------------|-----------------------|---------|
| Amber | refinement | |
| CYANA | structure calculation | |

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 | 1143 |
| Number of shifts mapped to atoms | 1143 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 74% |

6 Model quality i

6.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------------|-------------|----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.71±0.01 | 0±0/426 (0.0± 0.0%) | 1.01±0.04 | 1±1/574 (0.1± 0.2%) |
| 2 | B | 0.64±0.01 | 0±0/315 (0.0± 0.0%) | 0.97±0.04 | 0±0/432 (0.0± 0.1%) |
| All | All | 0.68 | 0/7410 (0.0%) | 0.99 | 8/10060 (0.1%) |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 49 | ARG | NE-CZ-NH1 | 8.30 | 124.45 | 120.30 | 2 | 3 |
| 2 | B | 288 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 | 5 | 2 |
| 1 | A | 58 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 | 5 | 2 |
| 1 | A | 49 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 | 2 | 1 |

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All | 7280 | 6860 | 6860 | - |

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

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|--------------|--------------|-------------|-------------|----|
| 1 | A | 52/61 (85%) | 38±1 (73±2%) | 11±2 (21±3%) | 3±1 (5±2%) | 3 | 23 |
| 2 | B | 41/62 (66%) | 24±2 (60±4%) | 12±2 (30±5%) | 4±2 (11±5%) | 1 | 8 |
| All | All | 930/1230 (76%) | 626 (67%) | 231 (25%) | 73 (8%) | 2 | 14 |

All 23 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 | 47 | SER | 10 |
| 2 | B | 290 | VAL | 8 |
| 1 | A | 43 | LYS | 7 |
| 2 | B | 296 | PRO | 7 |
| 2 | B | 289 | PRO | 5 |
| 1 | A | 57 | GLY | 4 |
| 2 | B | 309 | VAL | 4 |
| 2 | B | 325 | SER | 4 |
| 2 | B | 285 | ALA | 4 |
| 2 | B | 312 | GLN | 3 |
| 2 | B | 316 | ASP | 2 |
| 1 | A | 48 | LEU | 2 |
| 2 | B | 317 | GLN | 2 |
| 1 | A | 44 | ASP | 2 |
| 2 | B | 301 | LEU | 1 |
| 2 | B | 287 | SER | 1 |
| 2 | B | 323 | THR | 1 |
| 1 | A | 58 | ARG | 1 |
| 1 | A | 59 | VAL | 1 |
| 2 | B | 307 | ILE | 1 |
| 1 | A | 36 | GLN | 1 |
| 2 | B | 292 | GLN | 1 |
| 2 | B | 308 | SER | 1 |

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|--------------|-------------|-------------|----|
| 1 | A | 45/51 (88%) | 36±2 (80±4%) | 9±2 (20±4%) | 3 | 33 |
| 2 | B | 37/53 (70%) | 32±1 (85±2%) | 6±1 (15±2%) | 6 | 44 |
| All | All | 820/1040 (79%) | 674 (82%) | 146 (18%) | 4 | 38 |

All 45 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 | 17 | GLU | 10 |
| 1 | A | 48 | LEU | 10 |
| 2 | B | 323 | THR | 9 |
| 1 | A | 33 | LYS | 9 |
| 1 | A | 27 | TYR | 8 |
| 2 | B | 293 | THR | 8 |
| 2 | B | 301 | LEU | 6 |
| 1 | A | 58 | ARG | 5 |
| 2 | B | 310 | ASP | 5 |
| 1 | A | 18 | ASN | 5 |
| 2 | B | 309 | VAL | 5 |
| 1 | A | 41 | LEU | 5 |
| 1 | A | 34 | ASP | 4 |
| 1 | A | 35 | ILE | 4 |
| 1 | A | 13 | GLN | 4 |
| 1 | A | 49 | ARG | 4 |
| 1 | A | 56 | LEU | 3 |
| 1 | A | 50 | LYS | 3 |
| 2 | B | 302 | HIS | 3 |
| 2 | B | 316 | ASP | 3 |
| 1 | A | 11 | LEU | 3 |
| 2 | B | 312 | GLN | 2 |
| 2 | B | 292 | GLN | 2 |
| 1 | A | 10 | GLN | 2 |
| 2 | B | 315 | HIS | 2 |
| 2 | B | 317 | GLN | 2 |
| 1 | A | 20 | GLU | 2 |
| 2 | B | 300 | LYS | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | B | 320 | HIS | 1 |
| 1 | A | 36 | GLN | 1 |
| 1 | A | 52 | LYS | 1 |
| 1 | A | 46 | GLU | 1 |
| 2 | B | 291 | ASN | 1 |
| 2 | B | 286 | ASN | 1 |
| 1 | A | 51 | TYR | 1 |
| 1 | A | 24 | SER | 1 |
| 1 | A | 28 | LYS | 1 |
| 1 | A | 32 | GLN | 1 |
| 1 | A | 55 | LEU | 1 |
| 2 | B | 311 | SER | 1 |
| 2 | B | 318 | GLN | 1 |
| 2 | B | 288 | ARG | 1 |
| 2 | B | 313 | SER | 1 |
| 1 | A | 40 | GLU | 1 |
| 1 | A | 43 | LYS | 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 monosaccharides 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

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping i

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

| | |
|---|------|
| Total number of shifts | 1143 |
| Number of shifts mapped to atoms | 1143 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 118 | 0.15 ± 0.15 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 112 | 0.00 ± 0.25 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 105 | -1.28 ± 0.22 | Should be applied |

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 900 atoms were assigned a chemical shift out of a possible 1210. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 340/454 (75%) | 168/182 (92%) | 90/186 (48%) | 82/86 (95%) |
| Sidechain | 560/710 (79%) | 374/452 (83%) | 175/229 (76%) | 11/29 (38%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 0/46 (0%) | 0/24 (0%) | 0/18 (0%) | 0/4 (0%) |
| Overall | 900/1210 (74%) | 542/658 (82%) | 265/433 (61%) | 93/119 (78%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1143 atoms were assigned a chemical shift out of a possible 1572. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 440/607 (72%) | 217/246 (88%) | 118/246 (48%) | 105/115 (91%) |
| Sidechain | 703/907 (78%) | 467/575 (81%) | 224/290 (77%) | 12/42 (29%) |
| Aromatic | 0/58 (0%) | 0/30 (0%) | 0/23 (0%) | 0/5 (0%) |
| Overall | 1143/1572 (73%) | 684/851 (80%) | 342/559 (61%) | 117/162 (72%) |

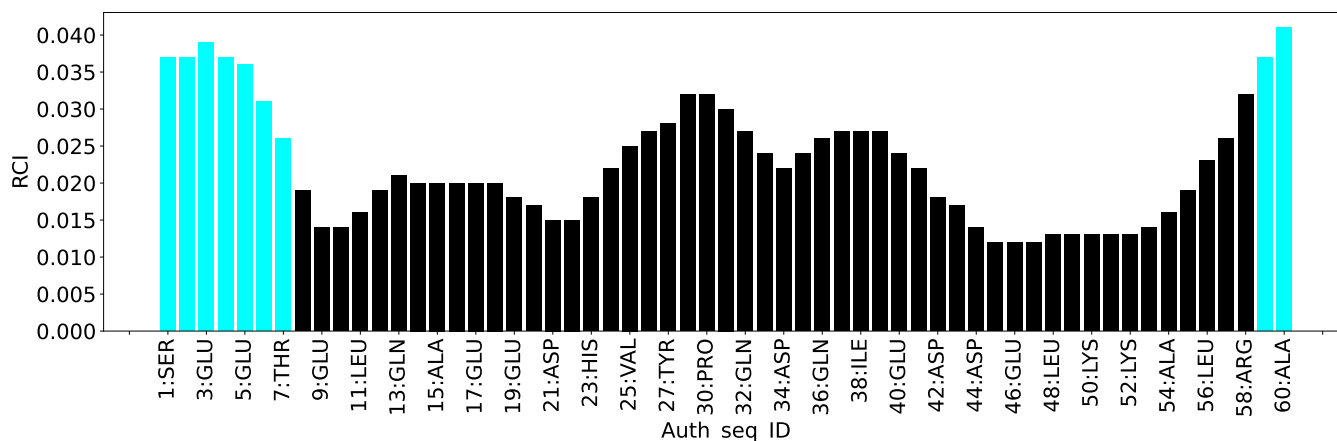
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

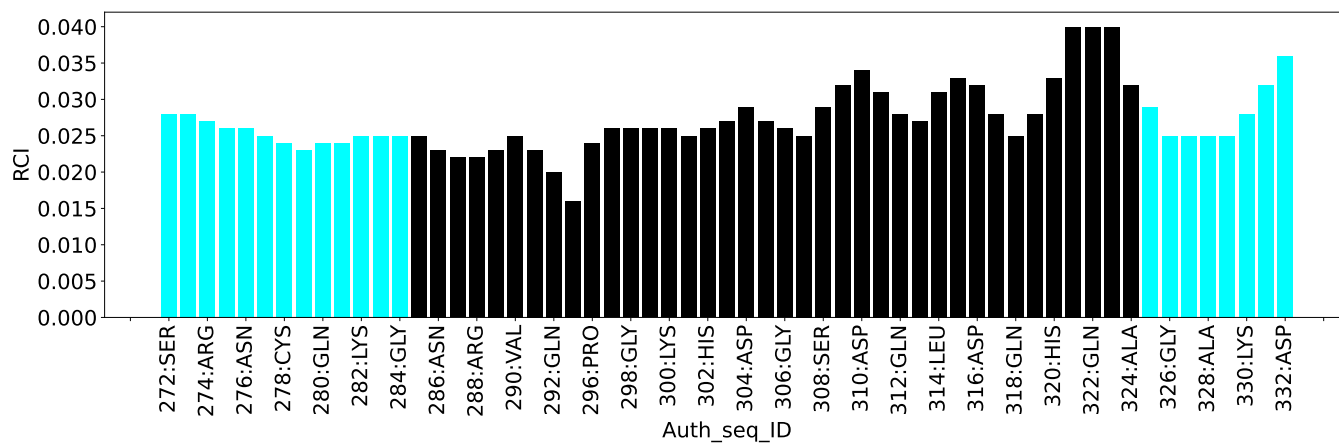
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 1398 |
| Intra-residue ($ i-j =0$) | 687 |
| Sequential ($ i-j =1$) | 471 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 179 |
| Long range ($ i-j \geq 5$) | 13 |
| Inter-chain | 48 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 11.4 |
| 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) | 48.8 | 0.2 |
| 0.2-0.5 (Medium) | 63.4 | 0.5 |
| >0.5 (Large) | 27.2 | 2.1 |

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

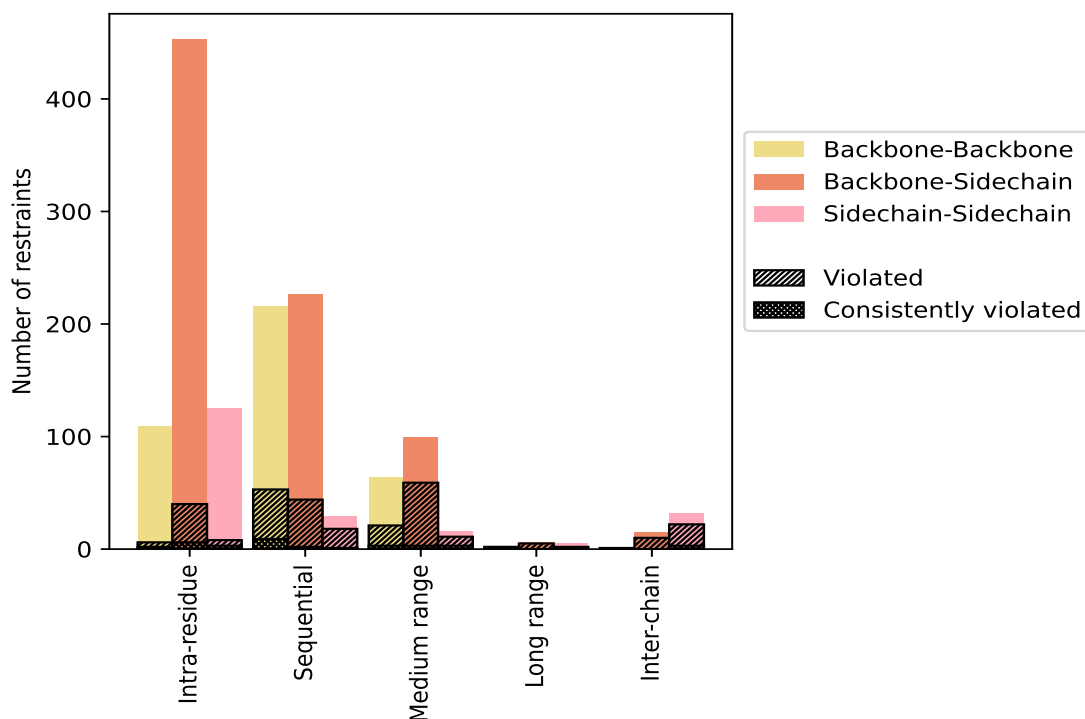
9.1 Summary of distance violations

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 687 | 49.1 | 54 | 7.9 | 3.9 | 11 | 1.6 | 0.8 |
| Backbone-Backbone | 109 | 7.8 | 6 | 5.5 | 0.4 | 2 | 1.8 | 0.1 |
| Backbone-Sidechain | 453 | 32.4 | 40 | 8.8 | 2.9 | 6 | 1.3 | 0.4 |
| Sidechain-Sidechain | 125 | 8.9 | 8 | 6.4 | 0.6 | 3 | 2.4 | 0.2 |
| Sequential ($i-j =1$) | 471 | 33.7 | 115 | 24.4 | 8.2 | 12 | 2.5 | 0.9 |
| Backbone-Backbone | 216 | 15.5 | 53 | 24.5 | 3.8 | 9 | 4.2 | 0.6 |
| Backbone-Sidechain | 226 | 16.2 | 44 | 19.5 | 3.1 | 2 | 0.9 | 0.1 |
| Sidechain-Sidechain | 29 | 2.1 | 18 | 62.1 | 1.3 | 1 | 3.4 | 0.1 |
| Medium range ($i-j >1$ & $i-j <5$) | 179 | 12.8 | 91 | 50.8 | 6.5 | 9 | 5.0 | 0.6 |
| Backbone-Backbone | 64 | 4.6 | 21 | 32.8 | 1.5 | 3 | 4.7 | 0.2 |
| Backbone-Sidechain | 99 | 7.1 | 59 | 59.6 | 4.2 | 3 | 3.0 | 0.2 |
| Sidechain-Sidechain | 16 | 1.1 | 11 | 68.8 | 0.8 | 3 | 18.8 | 0.2 |
| Long range ($i-j \geq 5$) | 13 | 0.9 | 9 | 69.2 | 0.6 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 2 | 0.1 | 2 | 100.0 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 6 | 0.4 | 5 | 83.3 | 0.4 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 5 | 0.4 | 2 | 40.0 | 0.1 | 0 | 0.0 | 0.0 |
| Inter-chain | 48 | 3.4 | 33 | 68.8 | 2.4 | 3 | 6.2 | 0.2 |
| Backbone-Backbone | 1 | 0.1 | 1 | 100.0 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 15 | 1.1 | 10 | 66.7 | 0.7 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 32 | 2.3 | 22 | 68.8 | 1.6 | 3 | 9.4 | 0.2 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1398 | 100.0 | 302 | 21.6 | 21.6 | 35 | 2.5 | 2.5 |
| Backbone-Backbone | 392 | 28.0 | 83 | 21.2 | 5.9 | 14 | 3.6 | 1.0 |
| Backbone-Sidechain | 799 | 57.2 | 158 | 19.8 | 11.3 | 11 | 1.4 | 0.8 |
| Sidechain-Sidechain | 207 | 14.8 | 61 | 29.5 | 4.4 | 10 | 4.8 | 0.7 |

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

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



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

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

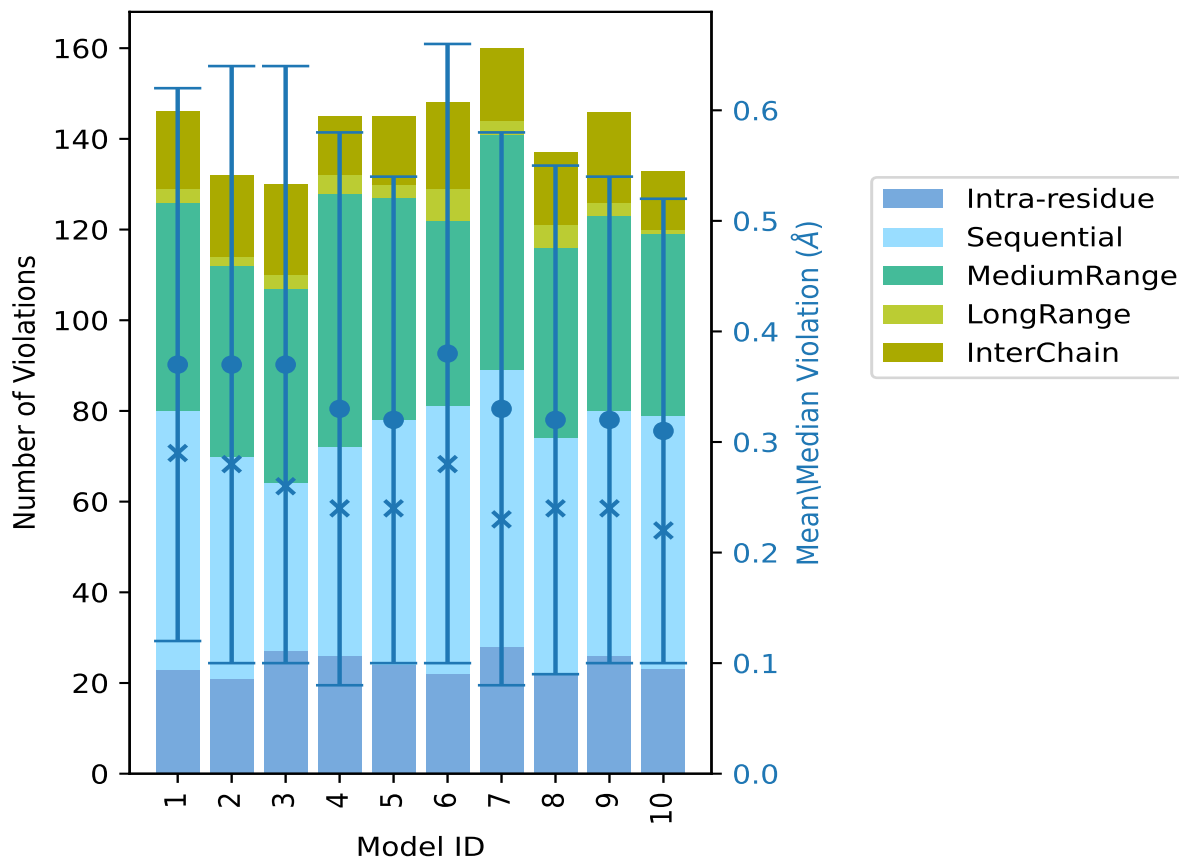
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 23 | 57 | 46 | 3 | 17 | 146 | 0.37 | 1.3 | 0.25 | 0.29 |
| 2 | 21 | 49 | 42 | 2 | 18 | 132 | 0.37 | 1.66 | 0.27 | 0.28 |
| 3 | 27 | 37 | 43 | 3 | 20 | 130 | 0.37 | 1.7 | 0.27 | 0.26 |
| 4 | 26 | 46 | 56 | 4 | 13 | 145 | 0.33 | 1.8 | 0.25 | 0.24 |
| 5 | 24 | 54 | 49 | 3 | 15 | 145 | 0.32 | 1.03 | 0.22 | 0.24 |
| 6 | 22 | 59 | 41 | 7 | 19 | 148 | 0.38 | 1.33 | 0.28 | 0.28 |
| 7 | 28 | 61 | 52 | 3 | 16 | 160 | 0.33 | 2.1 | 0.25 | 0.23 |
| 8 | 22 | 52 | 42 | 5 | 16 | 137 | 0.32 | 1.17 | 0.23 | 0.24 |
| 9 | 26 | 54 | 43 | 3 | 20 | 146 | 0.32 | 1.52 | 0.22 | 0.24 |
| 10 | 23 | 56 | 40 | 1 | 13 | 133 | 0.31 | 1.16 | 0.21 | 0.22 |

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

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, 1096(IR:633, SQ:356, MR:88, LR:4, IC:15) 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 | % |
| 14 | 31 | 17 | 2 | 5 | 69 | 1 | 10.0 |
| 12 | 16 | 11 | 1 | 4 | 44 | 2 | 20.0 |
| 4 | 7 | 2 | 2 | 4 | 19 | 3 | 30.0 |
| 4 | 9 | 13 | 1 | 4 | 31 | 4 | 40.0 |

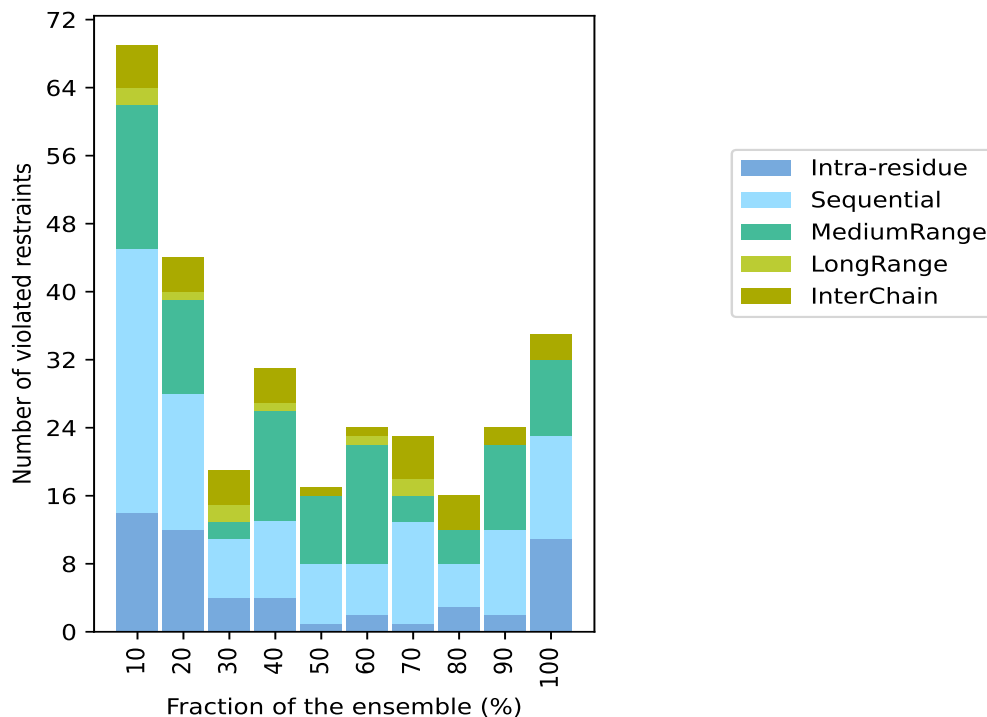
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 1 | 7 | 8 | 0 | 1 | 17 | 5 | 50.0 |
| 2 | 6 | 14 | 1 | 1 | 24 | 6 | 60.0 |
| 1 | 12 | 3 | 2 | 5 | 23 | 7 | 70.0 |
| 3 | 5 | 4 | 0 | 4 | 16 | 8 | 80.0 |
| 2 | 10 | 10 | 0 | 2 | 24 | 9 | 90.0 |
| 11 | 12 | 9 | 0 | 3 | 35 | 10 | 100.0 |

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

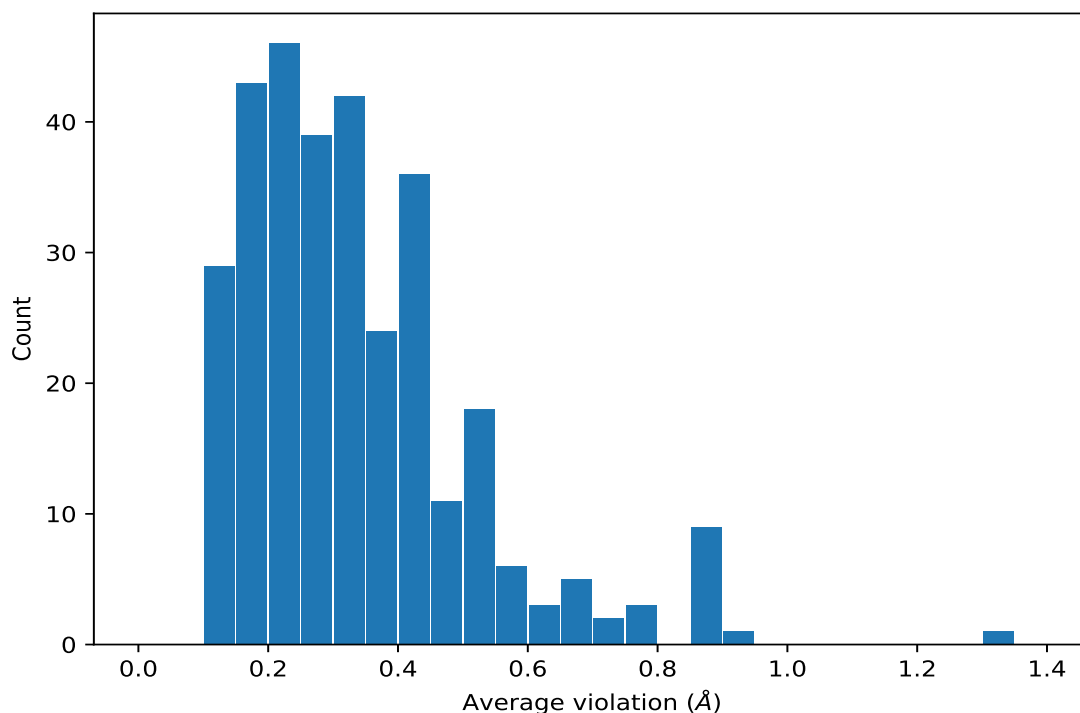
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 10 | 1.31 | 0.46 | 1.24 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 10 | 0.92 | 0.12 | 0.96 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 10 | 0.85 | 0.11 | 0.82 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 10 | 0.85 | 0.11 | 0.82 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 10 | 0.85 | 0.11 | 0.82 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 10 | 0.66 | 0.08 | 0.68 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 10 | 0.65 | 0.2 | 0.57 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 10 | 0.64 | 0.27 | 0.53 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 10 | 0.54 | 0.19 | 0.51 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 10 | 0.54 | 0.19 | 0.51 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 10 | 0.54 | 0.19 | 0.51 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 10 | 0.46 | 0.13 | 0.47 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 10 | 0.46 | 0.13 | 0.47 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 10 | 0.42 | 0.2 | 0.43 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 10 | 0.41 | 0.2 | 0.38 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 10 | 0.41 | 0.2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 10 | 0.41 | 0.2 | 0.38 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 10 | 0.34 | 0.24 | 0.3 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 10 | 0.33 | 0.12 | 0.33 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 10 | 0.32 | 0.11 | 0.33 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 10 | 0.32 | 0.11 | 0.33 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 10 | 0.3 | 0.05 | 0.29 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 10 | 0.28 | 0.05 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 10 | 0.28 | 0.05 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 10 | 0.28 | 0.05 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 10 | 0.28 | 0.05 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 10 | 0.28 | 0.05 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 10 | 0.28 | 0.05 | 0.26 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 10 | 0.24 | 0.01 | 0.24 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 10 | 0.22 | 0.0 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 10 | 0.22 | 0.0 | 0.22 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 10 | 0.21 | 0.02 | 0.21 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 10 | 0.21 | 0.02 | 0.21 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 10 | 0.21 | 0.02 | 0.21 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 10 | 0.21 | 0.0 | 0.21 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 10 | 0.2 | 0.03 | 0.2 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 10 | 0.19 | 0.01 | 0.19 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 10 | 0.19 | 0.02 | 0.19 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 10 | 0.18 | 0.02 | 0.18 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 10 | 0.18 | 0.02 | 0.18 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 10 | 0.18 | 0.03 | 0.2 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 10 | 0.18 | 0.03 | 0.2 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 10 | 0.17 | 0.03 | 0.18 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 10 | 0.17 | 0.03 | 0.18 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 10 | 0.14 | 0.03 | 0.14 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 9 | 0.86 | 0.23 | 0.86 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 9 | 0.86 | 0.23 | 0.86 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 9 | 0.86 | 0.23 | 0.86 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 9 | 0.86 | 0.23 | 0.86 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 9 | 0.86 | 0.23 | 0.86 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 9 | 0.86 | 0.23 | 0.86 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 9 | 0.78 | 0.25 | 0.75 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 9 | 0.78 | 0.25 | 0.75 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 9 | 0.71 | 0.15 | 0.71 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 9 | 0.68 | 0.41 | 0.71 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 9 | 0.64 | 0.25 | 0.56 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 9 | 0.62 | 0.36 | 0.56 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 9 | 0.55 | 0.2 | 0.51 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 9 | 0.54 | 0.17 | 0.55 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 9 | 0.54 | 0.17 | 0.55 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 9 | 0.54 | 0.17 | 0.55 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 9 | 0.53 | 0.23 | 0.56 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 9 | 0.48 | 0.16 | 0.46 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 9 | 0.35 | 0.17 | 0.28 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 9 | 0.35 | 0.17 | 0.28 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 9 | 0.35 | 0.17 | 0.28 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 9 | 0.35 | 0.11 | 0.31 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 9 | 0.35 | 0.11 | 0.31 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 9 | 0.31 | 0.17 | 0.25 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 9 | 0.31 | 0.17 | 0.25 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 9 | 0.31 | 0.17 | 0.25 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 9 | 0.26 | 0.08 | 0.3 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 9 | 0.25 | 0.14 | 0.21 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 9 | 0.24 | 0.08 | 0.22 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 9 | 0.22 | 0.02 | 0.22 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 9 | 0.21 | 0.02 | 0.22 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 9 | 0.19 | 0.03 | 0.19 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 9 | 0.19 | 0.03 | 0.19 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 9 | 0.12 | 0.02 | 0.12 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 8 | 0.69 | 0.28 | 0.63 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 8 | 0.54 | 0.16 | 0.59 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 8 | 0.54 | 0.16 | 0.59 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 8 | 0.54 | 0.16 | 0.59 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 8 | 0.41 | 0.12 | 0.38 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 8 | 0.39 | 0.11 | 0.4 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 8 | 0.36 | 0.13 | 0.38 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 8 | 0.36 | 0.13 | 0.38 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 8 | 0.36 | 0.11 | 0.38 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 8 | 0.36 | 0.11 | 0.38 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 8 | 0.36 | 0.11 | 0.38 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 8 | 0.34 | 0.03 | 0.34 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 8 | 0.29 | 0.01 | 0.3 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 8 | 0.29 | 0.01 | 0.3 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 8 | 0.29 | 0.17 | 0.24 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 8 | 0.29 | 0.17 | 0.24 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 8 | 0.29 | 0.17 | 0.24 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 8 | 0.24 | 0.06 | 0.26 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 8 | 0.23 | 0.08 | 0.21 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 8 | 0.16 | 0.02 | 0.15 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 8 | 0.15 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 8 | 0.15 | 0.03 | 0.15 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 7 | 0.66 | 0.27 | 0.66 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 7 | 0.54 | 0.3 | 0.44 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 7 | 0.5 | 0.35 | 0.49 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 7 | 0.49 | 0.24 | 0.44 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 7 | 0.44 | 0.13 | 0.47 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 7 | 0.44 | 0.13 | 0.47 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 7 | 0.44 | 0.17 | 0.36 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 7 | 0.44 | 0.17 | 0.36 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 7 | 0.44 | 0.17 | 0.36 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 7 | 0.4 | 0.19 | 0.36 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 7 | 0.4 | 0.19 | 0.36 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 7 | 0.4 | 0.19 | 0.36 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 7 | 0.36 | 0.13 | 0.31 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 7 | 0.36 | 0.13 | 0.31 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 7 | 0.35 | 0.23 | 0.28 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 7 | 0.35 | 0.13 | 0.42 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 7 | 0.35 | 0.13 | 0.42 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 7 | 0.35 | 0.13 | 0.42 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 7 | 0.33 | 0.16 | 0.28 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 7 | 0.31 | 0.11 | 0.25 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 7 | 0.3 | 0.14 | 0.25 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 7 | 0.3 | 0.14 | 0.25 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 7 | 0.3 | 0.14 | 0.25 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 7 | 0.26 | 0.09 | 0.25 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 7 | 0.24 | 0.01 | 0.24 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 7 | 0.18 | 0.03 | 0.18 |
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 7 | 0.18 | 0.02 | 0.18 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 7 | 0.18 | 0.02 | 0.18 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 7 | 0.14 | 0.02 | 0.13 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 7 | 0.14 | 0.02 | 0.14 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 7 | 0.14 | 0.02 | 0.14 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 6 | 0.47 | 0.36 | 0.32 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 6 | 0.46 | 0.16 | 0.43 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 6 | 0.46 | 0.16 | 0.43 |
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 6 | 0.43 | 0.19 | 0.51 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 6 | 0.42 | 0.18 | 0.4 |
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 6 | 0.42 | 0.18 | 0.4 |
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 6 | 0.35 | 0.14 | 0.31 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 6 | 0.35 | 0.14 | 0.31 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 6 | 0.34 | 0.18 | 0.26 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 6 | 0.34 | 0.18 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 6 | 0.32 | 0.08 | 0.32 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 6 | 0.32 | 0.08 | 0.32 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 6 | 0.32 | 0.08 | 0.32 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 6 | 0.31 | 0.16 | 0.3 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 6 | 0.3 | 0.05 | 0.32 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 6 | 0.3 | 0.16 | 0.24 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 6 | 0.3 | 0.16 | 0.24 |
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 6 | 0.24 | 0.06 | 0.25 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 6 | 0.24 | 0.06 | 0.25 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 6 | 0.23 | 0.08 | 0.2 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 6 | 0.23 | 0.08 | 0.2 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 6 | 0.19 | 0.04 | 0.19 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 6 | 0.19 | 0.02 | 0.18 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 6 | 0.19 | 0.02 | 0.18 |
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 6 | 0.15 | 0.04 | 0.14 |
| (1,713) | 1:58:A:ARG:HD2 | 1:57:A:GLY:HA2 | 5 | 0.47 | 0.13 | 0.47 |
| (1,714) | 1:57:A:GLY:HA2 | 1:58:A:ARG:HD2 | 5 | 0.47 | 0.13 | 0.47 |
| (1,1103) | 2:308:B:SER:HA | 2:311:B:SER:H | 5 | 0.45 | 0.19 | 0.47 |
| (1,1104) | 2:311:B:SER:H | 2:308:B:SER:HA | 5 | 0.45 | 0.19 | 0.47 |
| (1,635) | 1:50:A:LYS:HA | 1:53:A:GLU:HB2 | 5 | 0.43 | 0.23 | 0.28 |
| (1,1380) | 1:37:A:GLU:HB3 | 2:313:B:SER:H | 5 | 0.42 | 0.16 | 0.37 |
| (1,1331) | 2:329:B:LEU:HD11 | 2:330:B:LYS:HA | 5 | 0.33 | 0.16 | 0.26 |
| (1,1331) | 2:329:B:LEU:HD12 | 2:330:B:LYS:HA | 5 | 0.33 | 0.16 | 0.26 |
| (1,1331) | 2:329:B:LEU:HD13 | 2:330:B:LYS:HA | 5 | 0.33 | 0.16 | 0.26 |
| (1,690) | 1:52:A:LYS:HA | 1:56:A:LEU:HG | 5 | 0.33 | 0.21 | 0.28 |
| (1,691) | 1:56:A:LEU:HG | 1:52:A:LYS:HA | 5 | 0.33 | 0.21 | 0.28 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB1 | 5 | 0.29 | 0.1 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB2 | 5 | 0.29 | 0.1 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB3 | 5 | 0.29 | 0.1 | 0.27 |
| (1,169) | 1:15:A:ALA:HB1 | 1:18:A:ASN:H | 5 | 0.29 | 0.1 | 0.27 |
| (1,169) | 1:15:A:ALA:HB2 | 1:18:A:ASN:H | 5 | 0.29 | 0.1 | 0.27 |
| (1,169) | 1:15:A:ALA:HB3 | 1:18:A:ASN:H | 5 | 0.29 | 0.1 | 0.27 |
| (1,1006) | 2:305:B:SER:H | 2:302:B:HIS:HA | 5 | 0.28 | 0.1 | 0.24 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG21 | 5 | 0.28 | 0.2 | 0.22 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG22 | 5 | 0.28 | 0.2 | 0.22 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG23 | 5 | 0.28 | 0.2 | 0.22 |
| (1,1045) | 2:307:B:ILE:H | 2:307:B:ILE:HG13 | 5 | 0.21 | 0.15 | 0.14 |
| (1,1340) | 2:331:B:GLY:H | 2:330:B:LYS:HA | 5 | 0.13 | 0.02 | 0.13 |
| (1,1090) | 2:309:B:VAL:HA | 2:310:B:ASP:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,1091) | 2:310:B:ASP:H | 2:309:B:VAL:HA | 5 | 0.12 | 0.01 | 0.12 |
| (1,815) | 2:288:B:ARG:H | 2:285:B:ALA:HA | 4 | 0.74 | 0.34 | 0.73 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1105) | 2:308:B:SER:HB2 | 2:311:B:SER:H | 4 | 0.58 | 0.44 | 0.57 |
| (1,1106) | 2:311:B:SER:H | 2:308:B:SER:HB2 | 4 | 0.58 | 0.44 | 0.57 |
| (1,993) | 2:301:B:LEU:HD11 | 2:302:B:HIS:H | 4 | 0.57 | 0.19 | 0.61 |
| (1,993) | 2:301:B:LEU:HD12 | 2:302:B:HIS:H | 4 | 0.57 | 0.19 | 0.61 |
| (1,993) | 2:301:B:LEU:HD13 | 2:302:B:HIS:H | 4 | 0.57 | 0.19 | 0.61 |
| (1,1395) | 2:325:B:SER:HB2 | 1:52:A:LYS:HE2 | 4 | 0.43 | 0.27 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD21 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD22 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD23 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD21 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD22 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD23 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD21 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD22 | 4 | 0.42 | 0.17 | 0.48 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD23 | 4 | 0.42 | 0.17 | 0.48 |
| (1,851) | 2:289:B:PRO:HG3 | 2:291:B:ASN:H | 4 | 0.42 | 0.15 | 0.38 |
| (1,852) | 2:291:B:ASN:H | 2:289:B:PRO:HG3 | 4 | 0.42 | 0.15 | 0.38 |
| (1,1192) | 2:316:B:ASP:HB3 | 2:317:B:GLN:H | 4 | 0.35 | 0.16 | 0.33 |
| (1,1366) | 2:300:B:LYS:HD2 | 1:30:A:PRO:HD3 | 4 | 0.32 | 0.13 | 0.32 |
| (1,633) | 1:38:A:ILE:H | 1:53:A:GLU:HG3 | 4 | 0.25 | 0.12 | 0.2 |
| (1,220) | 1:19:A:GLU:HA | 1:22:A:GLU:HB3 | 4 | 0.23 | 0.15 | 0.18 |
| (1,422) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HB3 | 4 | 0.23 | 0.09 | 0.21 |
| (1,422) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HB3 | 4 | 0.23 | 0.09 | 0.21 |
| (1,422) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HB3 | 4 | 0.23 | 0.09 | 0.21 |
| (1,345) | 1:34:A:ASP:H | 1:31:A:ALA:HA | 4 | 0.22 | 0.12 | 0.21 |
| (1,479) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 4 | 0.22 | 0.1 | 0.21 |
| (1,480) | 1:40:A:GLU:HG2 | 1:43:A:LYS:HA | 4 | 0.22 | 0.1 | 0.21 |
| (1,481) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 4 | 0.22 | 0.1 | 0.21 |
| (1,571) | 1:49:A:ARG:H | 1:49:A:ARG:HD2 | 4 | 0.22 | 0.05 | 0.2 |
| (1,572) | 1:49:A:ARG:HD2 | 1:49:A:ARG:H | 4 | 0.22 | 0.05 | 0.2 |
| (1,36) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HB3 | 4 | 0.21 | 0.08 | 0.22 |
| (1,36) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HB3 | 4 | 0.21 | 0.08 | 0.22 |
| (1,36) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HB3 | 4 | 0.21 | 0.08 | 0.22 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB1 | 4 | 0.21 | 0.08 | 0.22 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB2 | 4 | 0.21 | 0.08 | 0.22 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB3 | 4 | 0.21 | 0.08 | 0.22 |
| (1,1379) | 2:309:B:VAL:HB | 1:46:A:GLU:H | 4 | 0.2 | 0.04 | 0.2 |
| (1,198) | 1:20:A:GLU:HA | 1:20:A:GLU:HB3 | 4 | 0.19 | 0.03 | 0.2 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB1 | 4 | 0.17 | 0.03 | 0.16 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB2 | 4 | 0.17 | 0.03 | 0.16 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB3 | 4 | 0.17 | 0.03 | 0.16 |
| (1,124) | 1:15:A:ALA:HB1 | 1:12:A:ALA:HA | 4 | 0.17 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,124) | 1:15:A:ALA:HB2 | 1:12:A:ALA:HA | 4 | 0.17 | 0.03 | 0.16 |
| (1,124) | 1:15:A:ALA:HB3 | 1:12:A:ALA:HA | 4 | 0.17 | 0.03 | 0.16 |
| (1,1249) | 2:323:B:THR:H | 2:321:B:THR:H | 4 | 0.16 | 0.05 | 0.16 |
| (1,315) | 1:28:A:LYS:H | 1:27:A:TYR:HA | 4 | 0.16 | 0.03 | 0.17 |
| (1,316) | 1:27:A:TYR:HA | 1:28:A:LYS:H | 4 | 0.16 | 0.03 | 0.17 |
| (1,103) | 1:13:A:GLN:HG3 | 1:14:A:ILE:H | 4 | 0.15 | 0.05 | 0.12 |
| (1,786) | 2:283:B:GLN:HA | 2:283:B:GLN:H | 4 | 0.12 | 0.02 | 0.11 |
| (1,429) | 1:38:A:ILE:HA | 1:39:A:GLN:H | 4 | 0.12 | 0.01 | 0.12 |
| (1,648) | 1:11:A:LEU:HG | 1:54:A:ALA:H | 3 | 0.78 | 0.24 | 0.71 |
| (1,1372) | 2:301:B:LEU:HG | 1:22:A:GLU:HA | 3 | 0.52 | 0.27 | 0.68 |
| (1,339) | 1:20:A:GLU:HA | 1:33:A:LYS:HD2 | 3 | 0.38 | 0.04 | 0.38 |
| (1,382) | 1:38:A:ILE:HD11 | 1:37:A:GLU:H | 3 | 0.34 | 0.12 | 0.27 |
| (1,382) | 1:38:A:ILE:HD12 | 1:37:A:GLU:H | 3 | 0.34 | 0.12 | 0.27 |
| (1,382) | 1:38:A:ILE:HD13 | 1:37:A:GLU:H | 3 | 0.34 | 0.12 | 0.27 |
| (1,773) | 2:280:B:GLN:H | 2:279:B:LYS:HD3 | 3 | 0.32 | 0.14 | 0.28 |
| (1,1357) | 1:13:A:GLN:HB3 | 2:288:B:ARG:H | 3 | 0.32 | 0.15 | 0.31 |
| (1,1238) | 2:321:B:THR:HG21 | 2:322:B:GLN:H | 3 | 0.31 | 0.2 | 0.21 |
| (1,1238) | 2:321:B:THR:HG22 | 2:322:B:GLN:H | 3 | 0.31 | 0.2 | 0.21 |
| (1,1238) | 2:321:B:THR:HG23 | 2:322:B:GLN:H | 3 | 0.31 | 0.2 | 0.21 |
| (1,1168) | 2:315:B:HIS:H | 2:313:B:SER:H | 3 | 0.3 | 0.09 | 0.34 |
| (1,368) | 1:33:A:LYS:HG2 | 1:36:A:GLN:HB3 | 3 | 0.28 | 0.14 | 0.22 |
| (1,1338) | 2:330:B:LYS:HD2 | 2:330:B:LYS:H | 3 | 0.27 | 0.12 | 0.25 |
| (1,1376) | 1:37:A:GLU:HA | 2:307:B:ILE:HA | 3 | 0.27 | 0.1 | 0.29 |
| (1,1351) | 1:14:A:ILE:HB | 2:277:B:SER:HB2 | 3 | 0.22 | 0.12 | 0.16 |
| (1,47) | 1:9:A:GLU:HB2 | 1:9:A:GLU:HA | 3 | 0.22 | 0.02 | 0.21 |
| (1,1323) | 2:328:B:ALA:H | 2:329:B:LEU:H | 3 | 0.2 | 0.06 | 0.22 |
| (1,1324) | 2:329:B:LEU:H | 2:328:B:ALA:H | 3 | 0.2 | 0.06 | 0.22 |
| (1,984) | 2:301:B:LEU:H | 2:301:B:LEU:HA | 3 | 0.13 | 0.02 | 0.14 |
| (1,70) | 1:11:A:LEU:HD21 | 1:11:A:LEU:HA | 3 | 0.12 | 0.02 | 0.13 |
| (1,70) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HA | 3 | 0.12 | 0.02 | 0.13 |
| (1,70) | 1:11:A:LEU:HD23 | 1:11:A:LEU:HA | 3 | 0.12 | 0.02 | 0.13 |
| (1,927) | 2:297:B:GLU:HA | 2:298:B:GLY:H | 3 | 0.12 | 0.02 | 0.12 |
| (1,928) | 2:298:B:GLY:H | 2:297:B:GLU:HA | 3 | 0.12 | 0.02 | 0.12 |
| (1,917) | 2:296:B:PRO:HG2 | 2:297:B:GLU:H | 2 | 0.54 | 0.05 | 0.54 |
| (1,918) | 2:297:B:GLU:H | 2:296:B:PRO:HG2 | 2 | 0.54 | 0.05 | 0.54 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB1 | 2 | 0.5 | 0.24 | 0.5 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB2 | 2 | 0.5 | 0.24 | 0.5 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB3 | 2 | 0.5 | 0.24 | 0.5 |
| (1,1195) | 2:317:B:GLN:H | 2:316:B:ASP:HB2 | 2 | 0.44 | 0.24 | 0.44 |
| (1,1133) | 2:312:B:GLN:HG2 | 2:312:B:GLN:H | 2 | 0.4 | 0.24 | 0.4 |
| (1,1134) | 2:312:B:GLN:H | 2:312:B:GLN:HG2 | 2 | 0.4 | 0.24 | 0.4 |
| (1,1373) | 2:301:B:LEU:HD21 | 1:39:A:GLN:HG2 | 2 | 0.4 | 0.05 | 0.4 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1373) | 2:301:B:LEU:HD22 | 1:39:A:GLN:HG2 | 2 | 0.4 | 0.05 | 0.4 |
| (1,1373) | 2:301:B:LEU:HD23 | 1:39:A:GLN:HG2 | 2 | 0.4 | 0.05 | 0.4 |
| (1,596) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 2 | 0.38 | 0.01 | 0.38 |
| (1,371) | 1:37:A:GLU:HB2 | 1:36:A:GLN:HA | 2 | 0.38 | 0.01 | 0.38 |
| (1,712) | 1:58:A:ARG:HG2 | 1:55:A:LEU:HA | 2 | 0.37 | 0.21 | 0.37 |
| (1,1145) | 2:313:B:SER:HB2 | 2:313:B:SER:H | 2 | 0.34 | 0.14 | 0.34 |
| (1,1146) | 2:313:B:SER:H | 2:313:B:SER:HB2 | 2 | 0.34 | 0.14 | 0.34 |
| (1,201) | 1:21:A:ASP:H | 1:18:A:ASN:HB3 | 2 | 0.31 | 0.03 | 0.31 |
| (1,627) | 1:52:A:LYS:H | 1:52:A:LYS:HB2 | 2 | 0.3 | 0.01 | 0.3 |
| (1,418) | 1:39:A:GLN:HB2 | 1:36:A:GLN:HA | 2 | 0.28 | 0.13 | 0.28 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD11 | 2 | 0.28 | 0.1 | 0.28 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD12 | 2 | 0.28 | 0.1 | 0.28 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD13 | 2 | 0.28 | 0.1 | 0.28 |
| (1,97) | 1:14:A:ILE:HD11 | 1:13:A:GLN:HB3 | 2 | 0.28 | 0.1 | 0.28 |
| (1,97) | 1:14:A:ILE:HD12 | 1:13:A:GLN:HB3 | 2 | 0.28 | 0.1 | 0.28 |
| (1,97) | 1:14:A:ILE:HD13 | 1:13:A:GLN:HB3 | 2 | 0.28 | 0.1 | 0.28 |
| (1,1388) | 1:41:A:LEU:HD11 | 2:320:B:HIS:H | 2 | 0.27 | 0.1 | 0.27 |
| (1,1388) | 1:41:A:LEU:HD12 | 2:320:B:HIS:H | 2 | 0.27 | 0.1 | 0.27 |
| (1,1388) | 1:41:A:LEU:HD13 | 2:320:B:HIS:H | 2 | 0.27 | 0.1 | 0.27 |
| (1,1367) | 2:300:B:LYS:HD2 | 1:33:A:LYS:HD3 | 2 | 0.26 | 0.05 | 0.26 |
| (1,659) | 1:10:A:GLN:H | 1:55:A:LEU:HA | 2 | 0.23 | 0.04 | 0.23 |
| (1,1147) | 2:314:B:LEU:HD11 | 2:313:B:SER:HB3 | 2 | 0.21 | 0.08 | 0.21 |
| (1,1147) | 2:314:B:LEU:HD12 | 2:313:B:SER:HB3 | 2 | 0.21 | 0.08 | 0.21 |
| (1,1147) | 2:314:B:LEU:HD13 | 2:313:B:SER:HB3 | 2 | 0.21 | 0.08 | 0.21 |
| (1,1109) | 2:310:B:ASP:HB3 | 2:311:B:SER:H | 2 | 0.2 | 0.05 | 0.2 |
| (1,526) | 1:47:A:SER:H | 1:46:A:GLU:H | 2 | 0.18 | 0.02 | 0.18 |
| (1,203) | 1:21:A:ASP:H | 1:19:A:GLU:HG2 | 2 | 0.18 | 0.04 | 0.18 |
| (1,778) | 2:279:B:LYS:HA | 2:282:B:LYS:H | 2 | 0.18 | 0.08 | 0.18 |
| (1,779) | 2:282:B:LYS:H | 2:279:B:LYS:HA | 2 | 0.18 | 0.08 | 0.18 |
| (1,1063) | 2:308:B:SER:HB2 | 2:308:B:SER:H | 2 | 0.17 | 0.0 | 0.17 |
| (1,1064) | 2:308:B:SER:H | 2:308:B:SER:HB2 | 2 | 0.17 | 0.0 | 0.17 |
| (1,95) | 1:11:A:LEU:HD11 | 1:14:A:ILE:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,95) | 1:11:A:LEU:HD12 | 1:14:A:ILE:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,95) | 1:11:A:LEU:HD13 | 1:14:A:ILE:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,348) | 1:34:A:ASP:H | 1:34:A:ASP:HA | 2 | 0.15 | 0.01 | 0.15 |
| (1,351) | 1:34:A:ASP:H | 1:34:A:ASP:HB2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,352) | 1:34:A:ASP:HB2 | 1:34:A:ASP:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,425) | 1:39:A:GLN:HG2 | 1:38:A:ILE:HA | 2 | 0.14 | 0.04 | 0.14 |
| (1,426) | 1:38:A:ILE:HA | 1:39:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,1299) | 2:326:B:GLY:HA2 | 2:327:B:GLN:H | 2 | 0.14 | 0.04 | 0.14 |
| (1,1300) | 2:327:B:GLN:H | 2:326:B:GLY:HA2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,1394) | 1:49:A:ARG:HD2 | 2:325:B:SER:HB3 | 2 | 0.14 | 0.02 | 0.14 |

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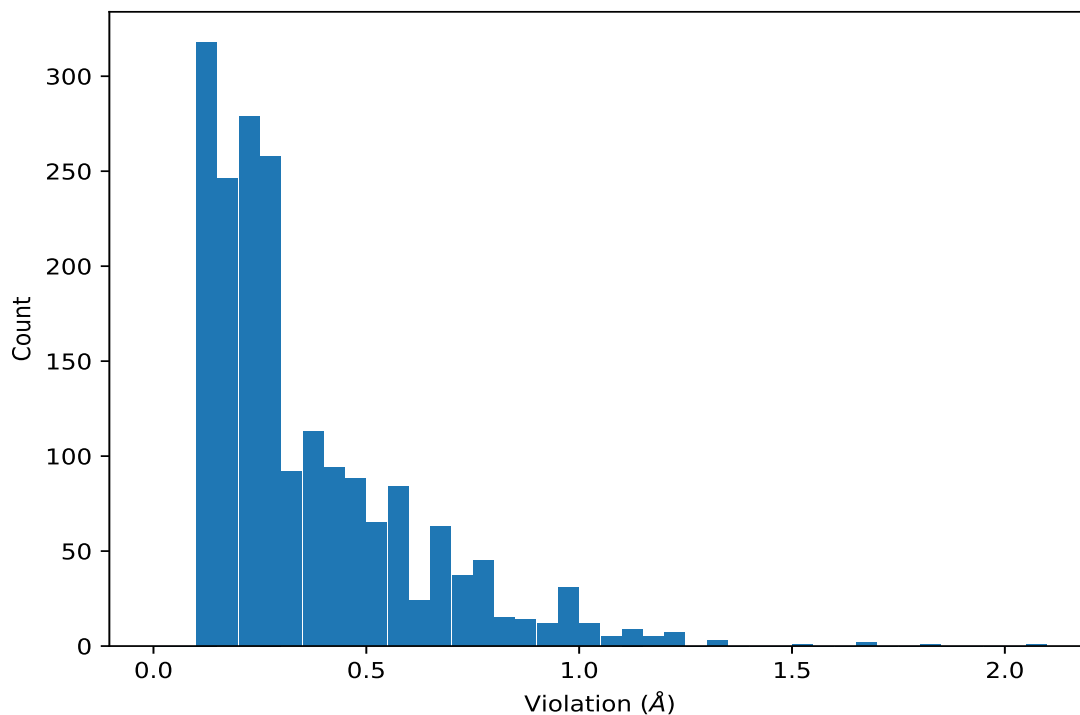
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1394) | 1:49:A:ARG:HD2 | 2:325:B:SER:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,599) | 1:51:A:TYR:HB3 | 1:48:A:LEU:HA | 2 | 0.13 | 0.01 | 0.13 |
| (1,600) | 1:48:A:LEU:HA | 1:51:A:TYR:HB3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,173) | 1:18:A:ASN:H | 1:18:A:ASN:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,354) | 1:35:A:ILE:H | 1:34:A:ASP:HA | 2 | 0.12 | 0.01 | 0.12 |
| (1,101) | 1:13:A:GLN:HA | 1:14:A:ILE:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,545) | 1:46:A:GLU:HA | 1:49:A:ARG:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1108) | 2:311:B:SER:H | 2:310:B:ASP:HA | 2 | 0.1 | 0.0 | 0.1 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 7 | 2.1 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 4 | 1.8 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 3 | 1.7 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 2 | 1.66 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 9 | 1.52 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 6 | 1.33 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 2 | 1.31 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 1 | 1.3 |
| (1,815) | 2:288:B:ARG:H | 2:285:B:ALA:HA | 1 | 1.24 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 6 | 1.22 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 6 | 1.22 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 6 | 1.22 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 6 | 1.22 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 6 | 1.22 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 6 | 1.22 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 8 | 1.17 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 6 | 1.17 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 8 | 1.17 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 4 | 1.16 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 10 | 1.16 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 9 | 1.13 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 9 | 1.13 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 9 | 1.13 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 9 | 1.13 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 9 | 1.13 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 9 | 1.13 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 6 | 1.12 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 6 | 1.12 |
| (1,648) | 1:11:A:LEU:HG | 1:54:A:ALA:H | 2 | 1.1 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 6 | 1.09 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 7 | 1.07 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 6 | 1.06 |
| (1,1106) | 2:311:B:SER:H | 2:308:B:SER:HB2 | 3 | 1.05 |
| (1,1105) | 2:308:B:SER:HB2 | 2:311:B:SER:H | 3 | 1.05 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 1 | 1.04 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 5 | 1.03 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 6 | 1.02 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 6 | 1.02 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 6 | 1.02 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 6 | 1.02 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 2 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 2 | 1.02 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 2 | 1.01 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 3 | 1.0 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 4 | 1.0 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 5 | 1.0 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 3 | 0.99 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 5 | 0.98 |
| (1,1106) | 2:311:B:SER:H | 2:308:B:SER:HB2 | 8 | 0.98 |
| (1,1105) | 2:308:B:SER:HB2 | 2:311:B:SER:H | 8 | 0.98 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 3 | 0.98 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 3 | 0.98 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 3 | 0.98 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 7 | 0.98 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 7 | 0.98 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 7 | 0.98 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 7 | 0.98 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 7 | 0.98 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 1 | 0.97 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 2 | 0.97 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 10 | 0.97 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 10 | 0.97 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 10 | 0.97 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 10 | 0.97 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 10 | 0.97 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 10 | 0.97 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 5 | 0.96 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 5 | 0.96 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 5 | 0.96 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 3 | 0.96 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 3 | 0.96 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 3 | 0.96 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 3 | 0.96 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 3 | 0.96 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 3 | 0.96 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 8 | 0.96 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 8 | 0.96 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 8 | 0.95 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 6 | 0.94 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 1 | 0.92 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 1 | 0.92 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 1 | 0.92 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 8 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 8 | 0.91 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 1 | 0.9 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 1 | 0.9 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 1 | 0.9 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 8 | 0.9 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 5 | 0.9 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 1 | 0.89 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 9 | 0.89 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 5 | 0.89 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 2 | 0.87 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 10 | 0.87 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 4 | 0.87 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 4 | 0.87 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 4 | 0.87 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 5 | 0.86 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 5 | 0.86 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 5 | 0.86 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 5 | 0.86 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 5 | 0.86 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 5 | 0.86 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 4 | 0.85 |
| (1,1173) | 2:314:B:LEU:HB2 | 2:315:B:HIS:H | 5 | 0.84 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 4 | 0.84 |
| (1,635) | 1:50:A:LYS:HA | 1:53:A:GLU:HB2 | 1 | 0.84 |
| (1,1354) | 1:13:A:GLN:HB3 | 2:284:B:GLY:HA2 | 6 | 0.83 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 6 | 0.83 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 5 | 0.82 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 6 | 0.81 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 3 | 0.81 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 7 | 0.81 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 1 | 0.8 |
| (1,993) | 2:301:B:LEU:HD11 | 2:302:B:HIS:H | 10 | 0.8 |
| (1,993) | 2:301:B:LEU:HD12 | 2:302:B:HIS:H | 10 | 0.8 |
| (1,993) | 2:301:B:LEU:HD13 | 2:302:B:HIS:H | 10 | 0.8 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 2 | 0.8 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 7 | 0.79 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 10 | 0.79 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 4 | 0.78 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 4 | 0.78 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 4 | 0.78 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 1 | 0.78 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 9 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 9 | 0.78 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 9 | 0.78 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 6 | 0.78 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 7 | 0.78 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 7 | 0.78 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 7 | 0.78 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 7 | 0.78 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 7 | 0.78 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 7 | 0.78 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 10 | 0.78 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 1 | 0.77 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 9 | 0.77 |
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 4 | 0.76 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 4 | 0.76 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 2 | 0.76 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 2 | 0.76 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 2 | 0.76 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 2 | 0.76 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 2 | 0.76 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 2 | 0.76 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 2 | 0.75 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 2 | 0.75 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 2 | 0.75 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 2 | 0.75 |
| (1,1372) | 2:301:B:LEU:HG | 1:22:A:GLU:HA | 4 | 0.75 |
| (1,1104) | 2:311:B:SER:H | 2:308:B:SER:HA | 1 | 0.75 |
| (1,1103) | 2:308:B:SER:HA | 2:311:B:SER:H | 1 | 0.75 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB1 | 1 | 0.75 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB2 | 1 | 0.75 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB3 | 1 | 0.75 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 5 | 0.75 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 5 | 0.75 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 5 | 0.75 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 10 | 0.75 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 10 | 0.75 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 10 | 0.75 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 3 | 0.75 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 3 | 0.75 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 7 | 0.74 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 3 | 0.74 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 3 | 0.74 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 1 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 3 | 0.73 |
| (1,815) | 2:288:B:ARG:H | 2:285:B:ALA:HA | 3 | 0.73 |
| (1,815) | 2:288:B:ARG:H | 2:285:B:ALA:HA | 9 | 0.73 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 2 | 0.73 |
| (1,1395) | 2:325:B:SER:HB2 | 1:52:A:LYS:HE2 | 3 | 0.72 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 7 | 0.72 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 7 | 0.72 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 7 | 0.72 |
| (1,1380) | 1:37:A:GLU:HB3 | 2:313:B:SER:H | 4 | 0.72 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 5 | 0.72 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 4 | 0.72 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 4 | 0.72 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 2 | 0.72 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 2 | 0.72 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 2 | 0.72 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 2 | 0.72 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 6 | 0.71 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 6 | 0.71 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 6 | 0.71 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 1 | 0.71 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 2 | 0.71 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 6 | 0.71 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 7 | 0.71 |
| (1,648) | 1:11:A:LEU:HG | 1:54:A:ALA:H | 6 | 0.71 |
| (1,536) | 1:48:A:LEU:HD11 | 1:45:A:ASP:HB3 | 8 | 0.71 |
| (1,536) | 1:48:A:LEU:HD12 | 1:45:A:ASP:HB3 | 8 | 0.71 |
| (1,536) | 1:48:A:LEU:HD13 | 1:45:A:ASP:HB3 | 8 | 0.71 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 1 | 0.71 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 1 | 0.71 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 1 | 0.71 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 3 | 0.71 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 3 | 0.71 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 3 | 0.71 |
| (1,1342) | 2:331:B:GLY:H | 2:330:B:LYS:H | 1 | 0.7 |
| (1,691) | 1:56:A:LEU:HG | 1:52:A:LYS:HA | 4 | 0.7 |
| (1,690) | 1:52:A:LYS:HA | 1:56:A:LEU:HG | 4 | 0.7 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 6 | 0.7 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 6 | 0.7 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 9 | 0.7 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 9 | 0.7 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 9 | 0.7 |
| (1,1395) | 2:325:B:SER:HB2 | 1:52:A:LYS:HE2 | 9 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 6 | 0.69 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 6 | 0.69 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 6 | 0.69 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 9 | 0.69 |
| (1,1195) | 2:317:B:GLN:H | 2:316:B:ASP:HB2 | 6 | 0.69 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 3 | 0.69 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 8 | 0.69 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 1 | 0.69 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 6 | 0.69 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 1 | 0.69 |
| (1,714) | 1:57:A:GLY:HA2 | 1:58:A:ARG:HD2 | 9 | 0.69 |
| (1,713) | 1:58:A:ARG:HD2 | 1:57:A:GLY:HA2 | 9 | 0.69 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 4 | 0.69 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 4 | 0.69 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 4 | 0.69 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 4 | 0.69 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 4 | 0.69 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 4 | 0.69 |
| (1,1372) | 2:301:B:LEU:HG | 1:22:A:GLU:HA | 2 | 0.68 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 10 | 0.68 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 6 | 0.68 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 9 | 0.68 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 3 | 0.67 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 3 | 0.67 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 3 | 0.67 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 5 | 0.67 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 2 | 0.67 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG21 | 8 | 0.67 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG22 | 8 | 0.67 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG23 | 8 | 0.67 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 4 | 0.67 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 4 | 0.67 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 4 | 0.67 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 9 | 0.66 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 1 | 0.66 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 1 | 0.66 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 1 | 0.66 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 5 | 0.66 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 6 | 0.66 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 1 | 0.66 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 1 | 0.66 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 1 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 10 | 0.65 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 2 | 0.65 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 2 | 0.65 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 1 | 0.65 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 6 | 0.65 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 6 | 0.65 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 6 | 0.65 |
| (1,852) | 2:291:B:ASN:H | 2:289:B:PRO:HG3 | 3 | 0.65 |
| (1,851) | 2:289:B:PRO:HG3 | 2:291:B:ASN:H | 3 | 0.65 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 10 | 0.65 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 5 | 0.65 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 5 | 0.65 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 5 | 0.64 |
| (1,1134) | 2:312:B:GLN:H | 2:312:B:GLN:HG2 | 1 | 0.64 |
| (1,1133) | 2:312:B:GLN:HG2 | 2:312:B:GLN:H | 1 | 0.64 |
| (1,993) | 2:301:B:LEU:HD11 | 2:302:B:HIS:H | 7 | 0.64 |
| (1,993) | 2:301:B:LEU:HD12 | 2:302:B:HIS:H | 7 | 0.64 |
| (1,993) | 2:301:B:LEU:HD13 | 2:302:B:HIS:H | 7 | 0.64 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 7 | 0.64 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 7 | 0.64 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 7 | 0.64 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 7 | 0.64 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 7 | 0.64 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 7 | 0.64 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 7 | 0.62 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 4 | 0.62 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 4 | 0.62 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 1 | 0.61 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 1 | 0.61 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 1 | 0.61 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 9 | 0.61 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 9 | 0.61 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 9 | 0.61 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 7 | 0.61 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 7 | 0.61 |
| (1,967) | 2:299:B:GLU:HB3 | 2:301:B:LEU:H | 3 | 0.61 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD21 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD22 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD23 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD21 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD22 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD23 | 2 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD21 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD22 | 2 | 0.6 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD23 | 2 | 0.6 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 3 | 0.6 |
| (1,1088) | 2:308:B:SER:H | 2:310:B:ASP:H | 7 | 0.6 |
| (1,381) | 1:38:A:ILE:HG21 | 1:35:A:ILE:H | 4 | 0.6 |
| (1,381) | 1:38:A:ILE:HG22 | 1:35:A:ILE:H | 4 | 0.6 |
| (1,381) | 1:38:A:ILE:HG23 | 1:35:A:ILE:H | 4 | 0.6 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 2 | 0.59 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 2 | 0.59 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 2 | 0.59 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 2 | 0.59 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 3 | 0.59 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 7 | 0.59 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 8 | 0.59 |
| (1,1238) | 2:321:B:THR:HG21 | 2:322:B:GLN:H | 7 | 0.59 |
| (1,1238) | 2:321:B:THR:HG22 | 2:322:B:GLN:H | 7 | 0.59 |
| (1,1238) | 2:321:B:THR:HG23 | 2:322:B:GLN:H | 7 | 0.59 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 3 | 0.59 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 3 | 0.59 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 3 | 0.59 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 5 | 0.59 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 5 | 0.59 |
| (1,918) | 2:297:B:GLU:H | 2:296:B:PRO:HG2 | 8 | 0.59 |
| (1,917) | 2:296:B:PRO:HG2 | 2:297:B:GLU:H | 8 | 0.59 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 10 | 0.59 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 10 | 0.59 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 7 | 0.59 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 7 | 0.59 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 7 | 0.59 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 10 | 0.59 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 10 | 0.59 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 10 | 0.59 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 2 | 0.58 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 7 | 0.58 |
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 7 | 0.58 |
| (1,993) | 2:301:B:LEU:HD11 | 2:302:B:HIS:H | 2 | 0.58 |
| (1,993) | 2:301:B:LEU:HD12 | 2:302:B:HIS:H | 2 | 0.58 |
| (1,993) | 2:301:B:LEU:HD13 | 2:302:B:HIS:H | 2 | 0.58 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 8 | 0.58 |
| (1,712) | 1:58:A:ARG:HG2 | 1:55:A:LEU:HA | 2 | 0.58 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 1 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 1 | 0.58 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 9 | 0.58 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 9 | 0.58 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 4 | 0.58 |
| (1,1381) | 1:38:A:ILE:HG21 | 2:316:B:ASP:HB2 | 9 | 0.57 |
| (1,1381) | 1:38:A:ILE:HG22 | 2:316:B:ASP:HB2 | 9 | 0.57 |
| (1,1381) | 1:38:A:ILE:HG23 | 2:316:B:ASP:HB2 | 9 | 0.57 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 5 | 0.57 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 5 | 0.57 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 5 | 0.57 |
| (1,1331) | 2:329:B:LEU:HD11 | 2:330:B:LYS:HA | 6 | 0.57 |
| (1,1331) | 2:329:B:LEU:HD12 | 2:330:B:LYS:HA | 6 | 0.57 |
| (1,1331) | 2:329:B:LEU:HD13 | 2:330:B:LYS:HA | 6 | 0.57 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 6 | 0.57 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 6 | 0.57 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 6 | 0.57 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 2 | 0.57 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 10 | 0.57 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 10 | 0.57 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 7 | 0.57 |
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 6 | 0.56 |
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 9 | 0.56 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 3 | 0.56 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 3 | 0.56 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 4 | 0.56 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 1 | 0.56 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 9 | 0.56 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 2 | 0.56 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 8 | 0.55 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 8 | 0.55 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 8 | 0.55 |
| (1,1370) | 2:300:B:LYS:HE2 | 1:35:A:ILE:HG21 | 1 | 0.55 |
| (1,1370) | 2:300:B:LYS:HE2 | 1:35:A:ILE:HG22 | 1 | 0.55 |
| (1,1370) | 2:300:B:LYS:HE2 | 1:35:A:ILE:HG23 | 1 | 0.55 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 4 | 0.55 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 3 | 0.55 |
| (1,1382) | 2:317:B:GLN:HB2 | 1:35:A:ILE:HB | 8 | 0.54 |
| (1,1192) | 2:316:B:ASP:HB3 | 2:317:B:GLN:H | 3 | 0.54 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 10 | 0.53 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 10 | 0.53 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 10 | 0.53 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 10 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 6 | 0.53 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 6 | 0.53 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 6 | 0.53 |
| (1,1104) | 2:311:B:SER:H | 2:308:B:SER:HA | 9 | 0.53 |
| (1,1103) | 2:308:B:SER:HA | 2:311:B:SER:H | 9 | 0.53 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 5 | 0.53 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 6 | 0.53 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 5 | 0.53 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 6 | 0.53 |
| (1,648) | 1:11:A:LEU:HG | 1:54:A:ALA:H | 8 | 0.53 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 10 | 0.53 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 2 | 0.53 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 1 | 0.53 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 1 | 0.53 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD21 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD22 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD23 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD21 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD22 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD23 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD21 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD22 | 7 | 0.52 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD23 | 7 | 0.52 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 5 | 0.52 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 8 | 0.52 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 9 | 0.52 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 9 | 0.52 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 9 | 0.52 |
| (1,1045) | 2:307:B:ILE:H | 2:307:B:ILE:HG13 | 10 | 0.52 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 3 | 0.52 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 1 | 0.52 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 8 | 0.52 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 5 | 0.51 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 9 | 0.51 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 9 | 0.51 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 9 | 0.51 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 9 | 0.51 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 6 | 0.51 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 1 | 0.51 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 5 | 0.51 |
| (1,382) | 1:38:A:ILE:HD11 | 1:37:A:GLU:H | 1 | 0.51 |
| (1,382) | 1:38:A:ILE:HD12 | 1:37:A:GLU:H | 1 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,382) | 1:38:A:ILE:HD13 | 1:37:A:GLU:H | 1 | 0.51 |
| (1,1357) | 1:13:A:GLN:HB3 | 2:288:B:ARG:H | 1 | 0.5 |
| (1,1250) | 2:323:B:THR:HB | 2:322:B:GLN:HB3 | 4 | 0.5 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 2 | 0.5 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 2 | 0.5 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 2 | 0.5 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 9 | 0.5 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 8 | 0.5 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 8 | 0.5 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 1 | 0.5 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 1 | 0.5 |
| (1,773) | 2:280:B:GLN:H | 2:279:B:LYS:HD3 | 9 | 0.5 |
| (1,664) | 1:52:A:LYS:HE2 | 1:55:A:LEU:HB3 | 6 | 0.5 |
| (1,635) | 1:50:A:LYS:HA | 1:53:A:GLU:HB2 | 9 | 0.5 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 7 | 0.5 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 7 | 0.5 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 3 | 0.5 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 6 | 0.49 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 6 | 0.49 |
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 6 | 0.49 |
| (1,918) | 2:297:B:GLU:H | 2:296:B:PRO:HG2 | 3 | 0.49 |
| (1,917) | 2:296:B:PRO:HG2 | 2:297:B:GLU:H | 3 | 0.49 |
| (1,610) | 1:52:A:LYS:HB2 | 1:49:A:ARG:HG2 | 1 | 0.49 |
| (1,609) | 1:49:A:ARG:HG2 | 1:52:A:LYS:HB2 | 1 | 0.49 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 1 | 0.49 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 4 | 0.49 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 4 | 0.49 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 4 | 0.49 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 8 | 0.49 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 9 | 0.49 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 1 | 0.49 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 2 | 0.49 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 1 | 0.49 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 2 | 0.49 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 10 | 0.49 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 10 | 0.49 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 10 | 0.49 |
| (1,1146) | 2:313:B:SER:H | 2:313:B:SER:HB2 | 4 | 0.48 |
| (1,1145) | 2:313:B:SER:HB2 | 2:313:B:SER:H | 4 | 0.48 |
| (1,714) | 1:57:A:GLY:HA2 | 1:58:A:ARG:HD2 | 5 | 0.48 |
| (1,713) | 1:58:A:ARG:HD2 | 1:57:A:GLY:HA2 | 5 | 0.48 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 3 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 3 | 0.48 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 3 | 0.48 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 9 | 0.48 |
| (1,169) | 1:15:A:ALA:HB1 | 1:18:A:ASN:H | 6 | 0.48 |
| (1,169) | 1:15:A:ALA:HB2 | 1:18:A:ASN:H | 6 | 0.48 |
| (1,169) | 1:15:A:ALA:HB3 | 1:18:A:ASN:H | 6 | 0.48 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB1 | 6 | 0.48 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB2 | 6 | 0.48 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB3 | 6 | 0.48 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 10 | 0.48 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 10 | 0.48 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 5 | 0.47 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 5 | 0.47 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 5 | 0.47 |
| (1,1192) | 2:316:B:ASP:HB3 | 2:317:B:GLN:H | 6 | 0.47 |
| (1,1104) | 2:311:B:SER:H | 2:308:B:SER:HA | 5 | 0.47 |
| (1,1103) | 2:308:B:SER:HA | 2:311:B:SER:H | 5 | 0.47 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 10 | 0.47 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 2 | 0.47 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 5 | 0.47 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 2 | 0.47 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 5 | 0.47 |
| (1,714) | 1:57:A:GLY:HA2 | 1:58:A:ARG:HD2 | 3 | 0.47 |
| (1,713) | 1:58:A:ARG:HD2 | 1:57:A:GLY:HA2 | 3 | 0.47 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 4 | 0.47 |
| (1,368) | 1:33:A:LYS:HG2 | 1:36:A:GLN:HB3 | 1 | 0.47 |
| (1,220) | 1:19:A:GLU:HA | 1:22:A:GLU:HB3 | 6 | 0.47 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 6 | 0.47 |
| (1,1366) | 2:300:B:LYS:HD2 | 1:30:A:PRO:HD3 | 4 | 0.46 |
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 3 | 0.46 |
| (1,1331) | 2:329:B:LEU:HD11 | 2:330:B:LYS:HA | 1 | 0.46 |
| (1,1331) | 2:329:B:LEU:HD12 | 2:330:B:LYS:HA | 1 | 0.46 |
| (1,1331) | 2:329:B:LEU:HD13 | 2:330:B:LYS:HA | 1 | 0.46 |
| (1,1254) | 2:322:B:GLN:HG2 | 2:323:B:THR:H | 10 | 0.46 |
| (1,1093) | 2:310:B:ASP:H | 2:309:B:VAL:HB | 4 | 0.46 |
| (1,852) | 2:291:B:ASN:H | 2:289:B:PRO:HG3 | 1 | 0.46 |
| (1,851) | 2:289:B:PRO:HG3 | 2:291:B:ASN:H | 1 | 0.46 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 7 | 0.46 |
| (1,714) | 1:57:A:GLY:HA2 | 1:58:A:ARG:HD2 | 6 | 0.46 |
| (1,713) | 1:58:A:ARG:HD2 | 1:57:A:GLY:HA2 | 6 | 0.46 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 10 | 0.46 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 10 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 9 | 0.46 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 9 | 0.46 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 2 | 0.46 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 6 | 0.46 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 6 | 0.46 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 2 | 0.46 |
| (1,1373) | 2:301:B:LEU:HD21 | 1:39:A:GLN:HG2 | 4 | 0.45 |
| (1,1373) | 2:301:B:LEU:HD22 | 1:39:A:GLN:HG2 | 4 | 0.45 |
| (1,1373) | 2:301:B:LEU:HD23 | 1:39:A:GLN:HG2 | 4 | 0.45 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 3 | 0.45 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 3 | 0.45 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 3 | 0.45 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 8 | 0.45 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 8 | 0.45 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 8 | 0.45 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 7 | 0.45 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 4 | 0.45 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 4 | 0.45 |
| (1,633) | 1:38:A:ILE:H | 1:53:A:GLU:HG3 | 8 | 0.45 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 1 | 0.45 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 4 | 0.45 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 6 | 0.44 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 10 | 0.44 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 10 | 0.44 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 10 | 0.44 |
| (1,1006) | 2:305:B:SER:H | 2:302:B:HIS:HA | 1 | 0.44 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 9 | 0.44 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 4 | 0.44 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 4 | 0.44 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 4 | 0.44 |
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 7 | 0.44 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 7 | 0.44 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 6 | 0.44 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 6 | 0.44 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 6 | 0.44 |
| (1,339) | 1:20:A:GLU:HA | 1:33:A:LYS:HD2 | 6 | 0.44 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 10 | 0.44 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD21 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD22 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD23 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD21 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD22 | 3 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD23 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD21 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD22 | 3 | 0.43 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD23 | 3 | 0.43 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 1 | 0.43 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 1 | 0.43 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 1 | 0.43 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 8 | 0.43 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 8 | 0.43 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 8 | 0.43 |
| (1,1366) | 2:300:B:LYS:HD2 | 1:30:A:PRO:HD3 | 8 | 0.43 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 1 | 0.43 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 1 | 0.43 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 1 | 0.43 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 1 | 0.43 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 5 | 0.43 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 5 | 0.43 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 3 | 0.43 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 3 | 0.43 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 3 | 0.43 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 5 | 0.42 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 5 | 0.42 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 5 | 0.42 |
| (1,1338) | 2:330:B:LYS:HD2 | 2:330:B:LYS:H | 5 | 0.42 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 10 | 0.42 |
| (1,691) | 1:56:A:LEU:HG | 1:52:A:LYS:HA | 2 | 0.42 |
| (1,690) | 1:52:A:LYS:HA | 1:56:A:LEU:HG | 2 | 0.42 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 1 | 0.42 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 1 | 0.42 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 1 | 0.42 |
| (1,418) | 1:39:A:GLN:HB2 | 1:36:A:GLN:HA | 9 | 0.42 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 10 | 0.42 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 10 | 0.42 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 4 | 0.42 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 4 | 0.42 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 5 | 0.42 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 5 | 0.42 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 5 | 0.42 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 8 | 0.41 |
| (1,1380) | 1:37:A:GLU:HB3 | 2:313:B:SER:H | 10 | 0.41 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 4 | 0.41 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 4 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 4 | 0.41 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 10 | 0.41 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 10 | 0.41 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 10 | 0.41 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 8 | 0.41 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 10 | 0.41 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 10 | 0.41 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 10 | 0.41 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 10 | 0.41 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 10 | 0.41 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 3 | 0.41 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 3 | 0.41 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 3 | 0.41 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 9 | 0.41 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 9 | 0.41 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 9 | 0.41 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 2 | 0.41 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 2 | 0.41 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 9 | 0.4 |
| (1,1241) | 2:322:B:GLN:HG2 | 2:322:B:GLN:HA | 4 | 0.4 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 1 | 0.4 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 1 | 0.4 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 1 | 0.4 |
| (1,925) | 2:298:B:GLY:H | 2:296:B:PRO:HB3 | 7 | 0.4 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 1 | 0.4 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 4 | 0.4 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 5 | 0.4 |
| (1,205) | 1:20:A:GLU:HB3 | 1:21:A:ASP:HB3 | 4 | 0.4 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 6 | 0.4 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 8 | 0.4 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 6 | 0.4 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 9 | 0.39 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 9 | 0.39 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 9 | 0.39 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 3 | 0.39 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 7 | 0.39 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 1 | 0.39 |
| (1,1168) | 2:315:B:HIS:H | 2:313:B:SER:H | 7 | 0.39 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 9 | 0.39 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 9 | 0.39 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 9 | 0.39 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 9 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 9 | 0.39 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 9 | 0.39 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 6 | 0.39 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 6 | 0.39 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 3 | 0.39 |
| (1,596) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 7 | 0.39 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 7 | 0.39 |
| (1,371) | 1:37:A:GLU:HB2 | 1:36:A:GLN:HA | 8 | 0.39 |
| (1,347) | 1:31:A:ALA:HB1 | 1:34:A:ASP:H | 1 | 0.39 |
| (1,347) | 1:31:A:ALA:HB2 | 1:34:A:ASP:H | 1 | 0.39 |
| (1,347) | 1:31:A:ALA:HB3 | 1:34:A:ASP:H | 1 | 0.39 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB1 | 1 | 0.39 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB2 | 1 | 0.39 |
| (1,346) | 1:34:A:ASP:H | 1:31:A:ALA:HB3 | 1 | 0.39 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 2 | 0.39 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 2 | 0.39 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 7 | 0.39 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 7 | 0.38 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 7 | 0.38 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 7 | 0.38 |
| (1,1376) | 1:37:A:GLU:HA | 2:307:B:ILE:HA | 2 | 0.38 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 4 | 0.38 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 8 | 0.38 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 8 | 0.38 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 8 | 0.38 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 9 | 0.38 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 9 | 0.38 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 9 | 0.38 |
| (1,1351) | 1:14:A:ILE:HB | 2:277:B:SER:HB2 | 8 | 0.38 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 4 | 0.38 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 1 | 0.38 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 1 | 0.38 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 1 | 0.38 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 7 | 0.38 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 7 | 0.38 |
| (1,596) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 5 | 0.38 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 3 | 0.38 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 3 | 0.38 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 6 | 0.38 |
| (1,422) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HB3 | 8 | 0.38 |
| (1,422) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HB3 | 8 | 0.38 |
| (1,422) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HB3 | 8 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,345) | 1:34:A:ASP:H | 1:31:A:ALA:HA | 6 | 0.38 |
| (1,339) | 1:20:A:GLU:HA | 1:33:A:LYS:HD2 | 9 | 0.38 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 3 | 0.38 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 3 | 0.38 |
| (1,97) | 1:14:A:ILE:HD11 | 1:13:A:GLN:HB3 | 10 | 0.38 |
| (1,97) | 1:14:A:ILE:HD12 | 1:13:A:GLN:HB3 | 10 | 0.38 |
| (1,97) | 1:14:A:ILE:HD13 | 1:13:A:GLN:HB3 | 10 | 0.38 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD11 | 10 | 0.38 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD12 | 10 | 0.38 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD13 | 10 | 0.38 |
| (1,1388) | 1:41:A:LEU:HD11 | 2:320:B:HIS:H | 6 | 0.37 |
| (1,1388) | 1:41:A:LEU:HD12 | 2:320:B:HIS:H | 6 | 0.37 |
| (1,1388) | 1:41:A:LEU:HD13 | 2:320:B:HIS:H | 6 | 0.37 |
| (1,1380) | 1:37:A:GLU:HB3 | 2:313:B:SER:H | 3 | 0.37 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 7 | 0.37 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 7 | 0.37 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 7 | 0.37 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 5 | 0.37 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 7 | 0.37 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 7 | 0.37 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 7 | 0.37 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 7 | 0.37 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 7 | 0.37 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 7 | 0.37 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 7 | 0.37 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 3 | 0.37 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 7 | 0.37 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 2 | 0.37 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 2 | 0.37 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 3 | 0.37 |
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 1 | 0.37 |
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 3 | 0.37 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 1 | 0.37 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 3 | 0.37 |
| (1,371) | 1:37:A:GLU:HB2 | 1:36:A:GLN:HA | 1 | 0.37 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 8 | 0.37 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 8 | 0.37 |
| (1,1380) | 1:37:A:GLU:HB3 | 2:313:B:SER:H | 9 | 0.36 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 10 | 0.36 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 10 | 0.36 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 10 | 0.36 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 10 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1334) | 2:330:B:LYS:H | 2:329:B:LEU:H | 2 | 0.36 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 2 | 0.36 |
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 10 | 0.36 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 6 | 0.36 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 6 | 0.36 |
| (1,1006) | 2:305:B:SER:H | 2:302:B:HIS:HA | 9 | 0.36 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 6 | 0.36 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 1 | 0.36 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 4 | 0.36 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 7 | 0.36 |
| (1,481) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 1 | 0.36 |
| (1,480) | 1:40:A:GLU:HG2 | 1:43:A:LYS:HA | 1 | 0.36 |
| (1,479) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 1 | 0.36 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 5 | 0.36 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 5 | 0.36 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 4 | 0.36 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 4 | 0.36 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 4 | 0.36 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 8 | 0.35 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 5 | 0.35 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 5 | 0.35 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 7 | 0.35 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 7 | 0.35 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 7 | 0.35 |
| (1,1373) | 2:301:B:LEU:HD21 | 1:39:A:GLN:HG2 | 2 | 0.34 |
| (1,1373) | 2:301:B:LEU:HD22 | 1:39:A:GLN:HG2 | 2 | 0.34 |
| (1,1373) | 2:301:B:LEU:HD23 | 1:39:A:GLN:HG2 | 2 | 0.34 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 7 | 0.34 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 7 | 0.34 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 7 | 0.34 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 2 | 0.34 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 2 | 0.34 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 2 | 0.34 |
| (1,1168) | 2:315:B:HIS:H | 2:313:B:SER:H | 1 | 0.34 |
| (1,1118) | 2:312:B:GLN:H | 2:309:B:VAL:HG11 | 7 | 0.34 |
| (1,1118) | 2:312:B:GLN:H | 2:309:B:VAL:HG12 | 7 | 0.34 |
| (1,1118) | 2:312:B:GLN:H | 2:309:B:VAL:HG13 | 7 | 0.34 |
| (1,1117) | 2:309:B:VAL:HG11 | 2:312:B:GLN:H | 7 | 0.34 |
| (1,1117) | 2:309:B:VAL:HG12 | 2:312:B:GLN:H | 7 | 0.34 |
| (1,1117) | 2:309:B:VAL:HG13 | 2:312:B:GLN:H | 7 | 0.34 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 9 | 0.34 |
| (1,935) | 2:299:B:GLU:HG2 | 2:298:B:GLY:HA2 | 7 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 6 | 0.34 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 6 | 0.34 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 6 | 0.34 |
| (1,201) | 1:21:A:ASP:H | 1:18:A:ASN:HB3 | 6 | 0.34 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 5 | 0.34 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 7 | 0.33 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 7 | 0.33 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 3 | 0.33 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 9 | 0.33 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 2 | 0.33 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 5 | 0.33 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 9 | 0.33 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 5 | 0.33 |
| (1,339) | 1:20:A:GLU:HA | 1:33:A:LYS:HD2 | 3 | 0.33 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 5 | 0.33 |
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 5 | 0.33 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 5 | 0.32 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 5 | 0.32 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 5 | 0.32 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 7 | 0.32 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 7 | 0.32 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 7 | 0.32 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 3 | 0.32 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 10 | 0.32 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 8 | 0.32 |
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 8 | 0.32 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 10 | 0.32 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 7 | 0.32 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 9 | 0.32 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 5 | 0.32 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 8 | 0.32 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 9 | 0.32 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 5 | 0.32 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 5 | 0.32 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 6 | 0.31 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 6 | 0.31 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 6 | 0.31 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 1 | 0.31 |
| (1,1367) | 2:300:B:LYS:HD2 | 1:33:A:LYS:HD3 | 8 | 0.31 |
| (1,1357) | 1:13:A:GLN:HB3 | 2:288:B:ARG:H | 9 | 0.31 |
| (1,1233) | 2:321:B:THR:HG21 | 2:322:B:GLN:HB2 | 7 | 0.31 |
| (1,1233) | 2:321:B:THR:HG22 | 2:322:B:GLN:HB2 | 7 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1233) | 2:321:B:THR:HG23 | 2:322:B:GLN:HB2 | 7 | 0.31 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 6 | 0.31 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 4 | 0.31 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 10 | 0.31 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 10 | 0.31 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 10 | 0.31 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 8 | 0.31 |
| (1,627) | 1:52:A:LYS:H | 1:52:A:LYS:HB2 | 6 | 0.31 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 3 | 0.31 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 2 | 0.31 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 9 | 0.31 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 9 | 0.31 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 1 | 0.31 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 1 | 0.31 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 8 | 0.31 |
| (1,166) | 1:18:A:ASN:HB2 | 1:15:A:ALA:HA | 9 | 0.31 |
| (1,165) | 1:15:A:ALA:HA | 1:18:A:ASN:HB2 | 9 | 0.31 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 2 | 0.31 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 2 | 0.31 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 2 | 0.31 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB1 | 7 | 0.31 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB2 | 7 | 0.31 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB3 | 7 | 0.31 |
| (1,36) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HB3 | 7 | 0.31 |
| (1,36) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HB3 | 7 | 0.31 |
| (1,36) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HB3 | 7 | 0.31 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 5 | 0.3 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 9 | 0.3 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 9 | 0.3 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 9 | 0.3 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 6 | 0.3 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 6 | 0.3 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 6 | 0.3 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 2 | 0.3 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 7 | 0.3 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 4 | 0.3 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 4 | 0.3 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 4 | 0.3 |
| (1,1341) | 2:330:B:LYS:HE2 | 2:331:B:GLY:H | 5 | 0.3 |
| (1,1307) | 2:328:B:ALA:H | 2:326:B:GLY:H | 5 | 0.3 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 8 | 0.3 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 5 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 5 | 0.3 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 2 | 0.3 |
| (1,1136) | 2:313:B:SER:H | 2:311:B:SER:H | 3 | 0.3 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 2 | 0.3 |
| (1,1135) | 2:311:B:SER:H | 2:313:B:SER:H | 3 | 0.3 |
| (1,852) | 2:291:B:ASN:H | 2:289:B:PRO:HG3 | 4 | 0.3 |
| (1,851) | 2:289:B:PRO:HG3 | 2:291:B:ASN:H | 4 | 0.3 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 2 | 0.3 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 6 | 0.3 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 9 | 0.3 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 9 | 0.3 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 10 | 0.3 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 2 | 0.3 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 2 | 0.3 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 2 | 0.3 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 8 | 0.3 |
| (1,345) | 1:34:A:ASP:H | 1:31:A:ALA:HA | 9 | 0.3 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 10 | 0.3 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 10 | 0.3 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 2 | 0.3 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 3 | 0.3 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 10 | 0.3 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 2 | 0.3 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 3 | 0.3 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 10 | 0.3 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 5 | 0.3 |
| (1,1376) | 1:37:A:GLU:HA | 2:307:B:ILE:HA | 3 | 0.29 |
| (1,1147) | 2:314:B:LEU:HD11 | 2:313:B:SER:HB3 | 6 | 0.29 |
| (1,1147) | 2:314:B:LEU:HD12 | 2:313:B:SER:HB3 | 6 | 0.29 |
| (1,1147) | 2:314:B:LEU:HD13 | 2:313:B:SER:HB3 | 6 | 0.29 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 6 | 0.29 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 6 | 0.29 |
| (1,572) | 1:49:A:ARG:HD2 | 1:49:A:ARG:H | 2 | 0.29 |
| (1,571) | 1:49:A:ARG:H | 1:49:A:ARG:HD2 | 2 | 0.29 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 6 | 0.29 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 6 | 0.29 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 4 | 0.29 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 4 | 0.29 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 4 | 0.29 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 4 | 0.29 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 4 | 0.29 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 4 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 10 | 0.29 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 1 | 0.29 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 9 | 0.29 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 9 | 0.29 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 9 | 0.29 |
| (1,1397) | 1:52:A:LYS:HG3 | 2:330:B:LYS:HG3 | 6 | 0.28 |
| (1,1368) | 2:300:B:LYS:HE2 | 1:33:A:LYS:HB2 | 9 | 0.28 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 6 | 0.28 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 6 | 0.28 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 6 | 0.28 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 4 | 0.28 |
| (1,1125) | 2:312:B:GLN:HG2 | 2:312:B:GLN:HA | 2 | 0.28 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 6 | 0.28 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 5 | 0.28 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 5 | 0.28 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 5 | 0.28 |
| (1,773) | 2:280:B:GLN:H | 2:279:B:LYS:HD3 | 10 | 0.28 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 8 | 0.28 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 8 | 0.28 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 8 | 0.28 |
| (1,691) | 1:56:A:LEU:HG | 1:52:A:LYS:HA | 1 | 0.28 |
| (1,690) | 1:52:A:LYS:HA | 1:56:A:LEU:HG | 1 | 0.28 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 9 | 0.28 |
| (1,635) | 1:50:A:LYS:HA | 1:53:A:GLU:HB2 | 4 | 0.28 |
| (1,627) | 1:52:A:LYS:H | 1:52:A:LYS:HB2 | 2 | 0.28 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 9 | 0.28 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 9 | 0.28 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 7 | 0.28 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 2 | 0.28 |
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 2 | 0.28 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 5 | 0.28 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 9 | 0.28 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 5 | 0.28 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 9 | 0.28 |
| (1,201) | 1:21:A:ASP:H | 1:18:A:ASN:HB3 | 3 | 0.28 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 6 | 0.28 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 6 | 0.28 |
| (1,169) | 1:15:A:ALA:HB1 | 1:18:A:ASN:H | 2 | 0.28 |
| (1,169) | 1:15:A:ALA:HB2 | 1:18:A:ASN:H | 2 | 0.28 |
| (1,169) | 1:15:A:ALA:HB3 | 1:18:A:ASN:H | 2 | 0.28 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB1 | 2 | 0.28 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB2 | 2 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB3 | 2 | 0.28 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB1 | 8 | 0.28 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB2 | 8 | 0.28 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB3 | 8 | 0.28 |
| (1,36) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HB3 | 8 | 0.28 |
| (1,36) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HB3 | 8 | 0.28 |
| (1,36) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HB3 | 8 | 0.28 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD11 | 3 | 0.27 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD12 | 3 | 0.27 |
| (1,1384) | 2:317:B:GLN:HB2 | 1:38:A:ILE:HD13 | 3 | 0.27 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 9 | 0.27 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 9 | 0.27 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 1 | 0.27 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 1 | 0.27 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 1 | 0.27 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 10 | 0.27 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 10 | 0.27 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 10 | 0.27 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 1 | 0.27 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 1 | 0.27 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 1 | 0.27 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 10 | 0.27 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 10 | 0.27 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 10 | 0.27 |
| (1,993) | 2:301:B:LEU:HD11 | 2:302:B:HIS:H | 6 | 0.27 |
| (1,993) | 2:301:B:LEU:HD12 | 2:302:B:HIS:H | 6 | 0.27 |
| (1,993) | 2:301:B:LEU:HD13 | 2:302:B:HIS:H | 6 | 0.27 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 8 | 0.27 |
| (1,815) | 2:288:B:ARG:H | 2:285:B:ALA:HA | 4 | 0.27 |
| (1,714) | 1:57:A:GLY:HA2 | 1:58:A:ARG:HD2 | 2 | 0.27 |
| (1,713) | 1:58:A:ARG:HD2 | 1:57:A:GLY:HA2 | 2 | 0.27 |
| (1,659) | 1:10:A:GLN:H | 1:55:A:LEU:HA | 6 | 0.27 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 5 | 0.27 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 5 | 0.27 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 5 | 0.27 |
| (1,382) | 1:38:A:ILE:HD11 | 1:37:A:GLU:H | 6 | 0.27 |
| (1,382) | 1:38:A:ILE:HD12 | 1:37:A:GLU:H | 6 | 0.27 |
| (1,382) | 1:38:A:ILE:HD13 | 1:37:A:GLU:H | 6 | 0.27 |
| (1,287) | 1:25:A:VAL:HG21 | 1:26:A:ASN:HB2 | 6 | 0.27 |
| (1,287) | 1:25:A:VAL:HG22 | 1:26:A:ASN:HB2 | 6 | 0.27 |
| (1,287) | 1:25:A:VAL:HG23 | 1:26:A:ASN:HB2 | 6 | 0.27 |
| (1,286) | 1:26:A:ASN:HB2 | 1:25:A:VAL:HG21 | 6 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,286) | 1:26:A:ASN:HB2 | 1:25:A:VAL:HG22 | 6 | 0.27 |
| (1,286) | 1:26:A:ASN:HB2 | 1:25:A:VAL:HG23 | 6 | 0.27 |
| (1,279) | 1:25:A:VAL:HB | 1:25:A:VAL:H | 7 | 0.27 |
| (1,278) | 1:25:A:VAL:H | 1:25:A:VAL:HB | 7 | 0.27 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 1 | 0.27 |
| (1,169) | 1:15:A:ALA:HB1 | 1:18:A:ASN:H | 7 | 0.27 |
| (1,169) | 1:15:A:ALA:HB2 | 1:18:A:ASN:H | 7 | 0.27 |
| (1,169) | 1:15:A:ALA:HB3 | 1:18:A:ASN:H | 7 | 0.27 |
| (1,169) | 1:15:A:ALA:HB1 | 1:18:A:ASN:H | 8 | 0.27 |
| (1,169) | 1:15:A:ALA:HB2 | 1:18:A:ASN:H | 8 | 0.27 |
| (1,169) | 1:15:A:ALA:HB3 | 1:18:A:ASN:H | 8 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB1 | 7 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB2 | 7 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB3 | 7 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB1 | 8 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB2 | 8 | 0.27 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB3 | 8 | 0.27 |
| (1,1379) | 2:309:B:VAL:HB | 1:46:A:GLU:H | 4 | 0.26 |
| (1,1331) | 2:329:B:LEU:HD11 | 2:330:B:LYS:HA | 5 | 0.26 |
| (1,1331) | 2:329:B:LEU:HD12 | 2:330:B:LYS:HA | 5 | 0.26 |
| (1,1331) | 2:329:B:LEU:HD13 | 2:330:B:LYS:HA | 5 | 0.26 |
| (1,1324) | 2:329:B:LEU:H | 2:328:B:ALA:H | 6 | 0.26 |
| (1,1323) | 2:328:B:ALA:H | 2:329:B:LEU:H | 6 | 0.26 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 7 | 0.26 |
| (1,1104) | 2:311:B:SER:H | 2:308:B:SER:HA | 8 | 0.26 |
| (1,1103) | 2:308:B:SER:HA | 2:311:B:SER:H | 8 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 2 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 2 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 2 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 3 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 3 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 3 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 5 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 5 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 5 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 6 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 6 | 0.26 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 6 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 2 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 2 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 2 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 3 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 3 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 5 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 5 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 5 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 6 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 6 | 0.26 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 6 | 0.26 |
| (1,969) | 2:299:B:GLU:HB2 | 2:301:B:LEU:H | 8 | 0.26 |
| (1,961) | 2:300:B:LYS:HG2 | 2:300:B:LYS:HA | 1 | 0.26 |
| (1,852) | 2:291:B:ASN:H | 2:289:B:PRO:HG3 | 2 | 0.26 |
| (1,851) | 2:289:B:PRO:HG3 | 2:291:B:ASN:H | 2 | 0.26 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB1 | 9 | 0.26 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB2 | 9 | 0.26 |
| (1,816) | 2:288:B:ARG:H | 2:285:B:ALA:HB3 | 9 | 0.26 |
| (1,779) | 2:282:B:LYS:H | 2:279:B:LYS:HA | 8 | 0.26 |
| (1,778) | 2:279:B:LYS:HA | 2:282:B:LYS:H | 8 | 0.26 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 5 | 0.26 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 5 | 0.26 |
| (1,635) | 1:50:A:LYS:HA | 1:53:A:GLU:HB2 | 10 | 0.26 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 4 | 0.26 |
| (1,481) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 4 | 0.26 |
| (1,480) | 1:40:A:GLU:HG2 | 1:43:A:LYS:HA | 4 | 0.26 |
| (1,479) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 4 | 0.26 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 9 | 0.26 |
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 9 | 0.26 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 8 | 0.26 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 8 | 0.26 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 2 | 0.26 |
| (1,148) | 1:13:A:GLN:HA | 1:17:A:GLU:H | 4 | 0.26 |
| (1,38) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HG2 | 5 | 0.26 |
| (1,38) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HG2 | 5 | 0.26 |
| (1,38) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HG2 | 5 | 0.26 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 9 | 0.25 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 9 | 0.25 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 9 | 0.25 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 2 | 0.25 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 2 | 0.25 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 2 | 0.25 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 10 | 0.25 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 10 | 0.25 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 10 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1338) | 2:330:B:LYS:HD2 | 2:330:B:LYS:H | 1 | 0.25 |
| (1,1331) | 2:329:B:LEU:HD11 | 2:330:B:LYS:HA | 4 | 0.25 |
| (1,1331) | 2:329:B:LEU:HD12 | 2:330:B:LYS:HA | 4 | 0.25 |
| (1,1331) | 2:329:B:LEU:HD13 | 2:330:B:LYS:HA | 4 | 0.25 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 3 | 0.25 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 3 | 0.25 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 6 | 0.25 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 5 | 0.25 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 1 | 0.25 |
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 1 | 0.25 |
| (1,1109) | 2:310:B:ASP:HB3 | 2:311:B:SER:H | 7 | 0.25 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 4 | 0.25 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 4 | 0.25 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 4 | 0.25 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 4 | 0.25 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 4 | 0.25 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 4 | 0.25 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 2 | 0.25 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 2 | 0.25 |
| (1,790) | 2:283:B:GLN:HG2 | 2:283:B:GLN:H | 7 | 0.25 |
| (1,660) | 1:11:A:LEU:HG | 1:55:A:LEU:HA | 2 | 0.25 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 8 | 0.25 |
| (1,635) | 1:50:A:LYS:HA | 1:53:A:GLU:HB2 | 7 | 0.25 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 1 | 0.25 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 6 | 0.25 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 7 | 0.25 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 9 | 0.25 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 5 | 0.25 |
| (1,382) | 1:38:A:ILE:HD11 | 1:37:A:GLU:H | 10 | 0.25 |
| (1,382) | 1:38:A:ILE:HD12 | 1:37:A:GLU:H | 10 | 0.25 |
| (1,382) | 1:38:A:ILE:HD13 | 1:37:A:GLU:H | 10 | 0.25 |
| (1,47) | 1:9:A:GLU:HB2 | 1:9:A:GLU:HA | 6 | 0.25 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 4 | 0.24 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 4 | 0.24 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 4 | 0.24 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 9 | 0.24 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 5 | 0.24 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 5 | 0.24 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 5 | 0.24 |
| (1,1249) | 2:323:B:THR:H | 2:321:B:THR:H | 4 | 0.24 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 10 | 0.24 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 7 | 0.24 |
| (1,1006) | 2:305:B:SER:H | 2:302:B:HIS:HA | 5 | 0.24 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 2 | 0.24 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 8 | 0.24 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 8 | 0.24 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 2 | 0.24 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 2 | 0.24 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 2 | 0.24 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 8 | 0.24 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 8 | 0.24 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 8 | 0.24 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 8 | 0.24 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 5 | 0.24 |
| (1,561) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HG3 | 1 | 0.24 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 3 | 0.24 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 5 | 0.24 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 8 | 0.24 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 9 | 0.24 |
| (1,560) | 1:49:A:ARG:HG3 | 1:49:A:ARG:HB2 | 10 | 0.24 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 1 | 0.24 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 2 | 0.24 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 3 | 0.24 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 4 | 0.24 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 5 | 0.24 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 8 | 0.24 |
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 8 | 0.24 |
| (1,268) | 1:25:A:VAL:HA | 1:25:A:VAL:HB | 6 | 0.24 |
| (1,103) | 1:13:A:GLN:HG3 | 1:14:A:ILE:H | 7 | 0.24 |
| (1,91) | 1:11:A:LEU:HD11 | 1:14:A:ILE:HA | 2 | 0.24 |
| (1,91) | 1:11:A:LEU:HD12 | 1:14:A:ILE:HA | 2 | 0.24 |
| (1,91) | 1:11:A:LEU:HD13 | 1:14:A:ILE:HA | 2 | 0.24 |
| (1,1380) | 1:37:A:GLU:HB3 | 2:313:B:SER:H | 7 | 0.23 |
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 7 | 0.23 |
| (1,1360) | 2:290:B:VAL:HG21 | 1:18:A:ASN:HB3 | 3 | 0.23 |
| (1,1360) | 2:290:B:VAL:HG22 | 1:18:A:ASN:HB3 | 3 | 0.23 |
| (1,1360) | 2:290:B:VAL:HG23 | 1:18:A:ASN:HB3 | 3 | 0.23 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 8 | 0.23 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 8 | 0.23 |
| (1,1199) | 2:317:B:GLN:HA | 2:317:B:GLN:HG2 | 7 | 0.23 |
| (1,1177) | 2:314:B:LEU:HD21 | 2:315:B:HIS:H | 7 | 0.23 |
| (1,1177) | 2:314:B:LEU:HD22 | 2:315:B:HIS:H | 7 | 0.23 |
| (1,1177) | 2:314:B:LEU:HD23 | 2:315:B:HIS:H | 7 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1171) | 2:314:B:LEU:HB3 | 2:315:B:HIS:H | 1 | 0.23 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 3 | 0.23 |
| (1,1104) | 2:311:B:SER:H | 2:308:B:SER:HA | 4 | 0.23 |
| (1,1103) | 2:308:B:SER:HA | 2:311:B:SER:H | 4 | 0.23 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG21 | 8 | 0.23 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG22 | 8 | 0.23 |
| (1,1049) | 2:307:B:ILE:H | 2:307:B:ILE:HG23 | 8 | 0.23 |
| (1,1048) | 2:307:B:ILE:HG21 | 2:307:B:ILE:H | 8 | 0.23 |
| (1,1048) | 2:307:B:ILE:HG22 | 2:307:B:ILE:H | 8 | 0.23 |
| (1,1048) | 2:307:B:ILE:HG23 | 2:307:B:ILE:H | 8 | 0.23 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 4 | 0.23 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 6 | 0.23 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 1 | 0.23 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 3 | 0.23 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 1 | 0.23 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 3 | 0.23 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 8 | 0.23 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 10 | 0.23 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 7 | 0.23 |
| (1,633) | 1:38:A:ILE:H | 1:53:A:GLU:HG3 | 7 | 0.23 |
| (1,611) | 1:52:A:LYS:HD3 | 1:49:A:ARG:HA | 6 | 0.23 |
| (1,586) | 1:50:A:LYS:HE2 | 1:50:A:LYS:HD2 | 3 | 0.23 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 8 | 0.23 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 9 | 0.23 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 5 | 0.23 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 9 | 0.23 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 7 | 0.23 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 7 | 0.23 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG21 | 1 | 0.23 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG22 | 1 | 0.23 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG23 | 1 | 0.23 |
| (1,236) | 1:23:A:HIS:H | 1:22:A:GLU:HG3 | 10 | 0.23 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 8 | 0.23 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 9 | 0.23 |
| (1,220) | 1:19:A:GLU:HA | 1:22:A:GLU:HB3 | 3 | 0.23 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 3 | 0.22 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 3 | 0.22 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 3 | 0.22 |
| (1,1389) | 1:52:A:LYS:HG3 | 2:320:B:HIS:HB3 | 8 | 0.22 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 8 | 0.22 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 8 | 0.22 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1350) | 2:332:B:ASP:H | 2:331:B:GLY:HA2 | 8 | 0.22 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 9 | 0.22 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 9 | 0.22 |
| (1,1324) | 2:329:B:LEU:H | 2:328:B:ALA:H | 5 | 0.22 |
| (1,1323) | 2:328:B:ALA:H | 2:329:B:LEU:H | 5 | 0.22 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 4 | 0.22 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 4 | 0.22 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 2 | 0.22 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 8 | 0.22 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 3 | 0.22 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 7 | 0.22 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 10 | 0.22 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 4 | 0.22 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 7 | 0.22 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 7 | 0.22 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 7 | 0.22 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 7 | 0.22 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 9 | 0.22 |
| (1,502) | 1:45:A:ASP:HB3 | 1:45:A:ASP:HA | 10 | 0.22 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 3 | 0.22 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 8 | 0.22 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 3 | 0.22 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 8 | 0.22 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 10 | 0.22 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 9 | 0.22 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 9 | 0.22 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 9 | 0.22 |
| (1,368) | 1:33:A:LYS:HG2 | 1:36:A:GLN:HB3 | 4 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 1 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 2 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 3 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 4 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 5 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 6 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 7 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 8 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 9 | 0.22 |
| (1,325) | 1:30:A:PRO:HG2 | 1:30:A:PRO:HD3 | 10 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 1 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 2 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 3 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 5 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 6 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 7 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 8 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 9 | 0.22 |
| (1,324) | 1:30:A:PRO:HD3 | 1:30:A:PRO:HG2 | 10 | 0.22 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG21 | 4 | 0.22 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG22 | 4 | 0.22 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG23 | 4 | 0.22 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 6 | 0.22 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 2 | 0.22 |
| (1,203) | 1:21:A:ASP:H | 1:19:A:GLU:HG2 | 6 | 0.22 |
| (1,198) | 1:20:A:GLU:HA | 1:20:A:GLU:HB3 | 7 | 0.22 |
| (1,124) | 1:15:A:ALA:HB1 | 1:12:A:ALA:HA | 5 | 0.22 |
| (1,124) | 1:15:A:ALA:HB2 | 1:12:A:ALA:HA | 5 | 0.22 |
| (1,124) | 1:15:A:ALA:HB3 | 1:12:A:ALA:HA | 5 | 0.22 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB1 | 5 | 0.22 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB2 | 5 | 0.22 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB3 | 5 | 0.22 |
| (1,1379) | 2:309:B:VAL:HB | 1:46:A:GLU:H | 6 | 0.21 |
| (1,1366) | 2:300:B:LYS:HD2 | 1:30:A:PRO:HD3 | 1 | 0.21 |
| (1,1238) | 2:321:B:THR:HG21 | 2:322:B:GLN:H | 10 | 0.21 |
| (1,1238) | 2:321:B:THR:HG22 | 2:322:B:GLN:H | 10 | 0.21 |
| (1,1238) | 2:321:B:THR:HG23 | 2:322:B:GLN:H | 10 | 0.21 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 7 | 0.21 |
| (1,1212) | 2:317:B:GLN:HG2 | 2:318:B:GLN:H | 9 | 0.21 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 1 | 0.21 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 6 | 0.21 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 1 | 0.21 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 10 | 0.21 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 2 | 0.21 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 6 | 0.21 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 9 | 0.21 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 2 | 0.21 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 6 | 0.21 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 9 | 0.21 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 4 | 0.21 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 9 | 0.21 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 4 | 0.21 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 9 | 0.21 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 4 | 0.21 |
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 4 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 1 | 0.21 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 2 | 0.21 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 6 | 0.21 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 7 | 0.21 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 8 | 0.21 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 9 | 0.21 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 9 | 0.21 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 9 | 0.21 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 10 | 0.21 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 9 | 0.21 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 9 | 0.21 |
| (1,748) | 2:274:B:ARG:HA | 2:273:B:LYS:HD2 | 8 | 0.21 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 5 | 0.21 |
| (1,572) | 1:49:A:ARG:HD2 | 1:49:A:ARG:H | 3 | 0.21 |
| (1,571) | 1:49:A:ARG:H | 1:49:A:ARG:HD2 | 3 | 0.21 |
| (1,422) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HB3 | 4 | 0.21 |
| (1,422) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HB3 | 4 | 0.21 |
| (1,422) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HB3 | 4 | 0.21 |
| (1,422) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HB3 | 10 | 0.21 |
| (1,422) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HB3 | 10 | 0.21 |
| (1,422) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HB3 | 10 | 0.21 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 3 | 0.21 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 2 | 0.21 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 6 | 0.21 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 2 | 0.21 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 6 | 0.21 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 2 | 0.21 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 3 | 0.21 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 7 | 0.21 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 9 | 0.21 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 10 | 0.21 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 9 | 0.21 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 1 | 0.21 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 5 | 0.21 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 6 | 0.21 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 10 | 0.21 |
| (1,198) | 1:20:A:GLU:HA | 1:20:A:GLU:HB3 | 3 | 0.21 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 2 | 0.21 |
| (1,150) | 1:14:A:ILE:HG13 | 1:17:A:GLU:HG3 | 8 | 0.21 |
| (1,149) | 1:17:A:GLU:HG3 | 1:14:A:ILE:HG13 | 8 | 0.21 |
| (1,47) | 1:9:A:GLU:HB2 | 1:9:A:GLU:HA | 7 | 0.21 |
| (1,1379) | 2:309:B:VAL:HB | 1:46:A:GLU:H | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1367) | 2:300:B:LYS:HD2 | 1:33:A:LYS:HD3 | 3 | 0.2 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 10 | 0.2 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 10 | 0.2 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 6 | 0.2 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 6 | 0.2 |
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 7 | 0.2 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 10 | 0.2 |
| (1,1195) | 2:317:B:GLN:H | 2:316:B:ASP:HB2 | 2 | 0.2 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 8 | 0.2 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 8 | 0.2 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 2 | 0.2 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 1 | 0.2 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 7 | 0.2 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 10 | 0.2 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 1 | 0.2 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 7 | 0.2 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 10 | 0.2 |
| (1,1006) | 2:305:B:SER:H | 2:302:B:HIS:HA | 7 | 0.2 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 4 | 0.2 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 5 | 0.2 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 10 | 0.2 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 5 | 0.2 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 10 | 0.2 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 3 | 0.2 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 4 | 0.2 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 5 | 0.2 |
| (1,908) | 2:296:B:PRO:HG2 | 2:296:B:PRO:HD3 | 10 | 0.2 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 4 | 0.2 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 4 | 0.2 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 4 | 0.2 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 6 | 0.2 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 6 | 0.2 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 6 | 0.2 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 5 | 0.2 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 5 | 0.2 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 10 | 0.2 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 7 | 0.2 |
| (1,572) | 1:49:A:ARG:HD2 | 1:49:A:ARG:H | 6 | 0.2 |
| (1,571) | 1:49:A:ARG:H | 1:49:A:ARG:HD2 | 6 | 0.2 |
| (1,526) | 1:47:A:SER:H | 1:46:A:GLU:H | 9 | 0.2 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 7 | 0.2 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 7 | 0.2 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 8 | 0.2 |
| (1,420) | 1:39:A:GLN:H | 1:36:A:GLN:HB2 | 8 | 0.2 |
| (1,359) | 1:35:A:ILE:H | 1:34:A:ASP:H | 8 | 0.2 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 1 | 0.2 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 4 | 0.2 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 5 | 0.2 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 6 | 0.2 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 1 | 0.2 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 5 | 0.2 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 7 | 0.2 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 7 | 0.2 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 3 | 0.2 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 4 | 0.2 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 7 | 0.2 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 8 | 0.2 |
| (1,139) | 1:16:A:ALA:H | 1:13:A:GLN:HG2 | 3 | 0.2 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 7 | 0.19 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 9 | 0.19 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 1 | 0.19 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 1 | 0.19 |
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 2 | 0.19 |
| (1,1192) | 2:316:B:ASP:HB3 | 2:317:B:GLN:H | 4 | 0.19 |
| (1,1192) | 2:316:B:ASP:HB3 | 2:317:B:GLN:H | 9 | 0.19 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 5 | 0.19 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 10 | 0.19 |
| (1,1161) | 2:314:B:LEU:H | 2:314:B:LEU:HB3 | 10 | 0.19 |
| (1,1146) | 2:313:B:SER:H | 2:313:B:SER:HB2 | 10 | 0.19 |
| (1,1145) | 2:313:B:SER:HB2 | 2:313:B:SER:H | 10 | 0.19 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 3 | 0.19 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 4 | 0.19 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 5 | 0.19 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 8 | 0.19 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 9 | 0.19 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 1 | 0.19 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 5 | 0.19 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 8 | 0.19 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 5 | 0.19 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 2 | 0.19 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 2 | 0.19 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 5 | 0.19 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 7 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 5 | 0.19 |
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 7 | 0.19 |
| (1,892) | 2:293:B:THR:H | 2:291:B:ASN:HA | 9 | 0.19 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 1 | 0.19 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 9 | 0.19 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 1 | 0.19 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 9 | 0.19 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 1 | 0.19 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 6 | 0.19 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 8 | 0.19 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 1 | 0.19 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 6 | 0.19 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 8 | 0.19 |
| (1,659) | 1:10:A:GLN:H | 1:55:A:LEU:HA | 4 | 0.19 |
| (1,555) | 1:49:A:ARG:HD2 | 1:49:A:ARG:HB2 | 2 | 0.19 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 4 | 0.19 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG21 | 1 | 0.19 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG22 | 1 | 0.19 |
| (1,455) | 1:41:A:LEU:H | 1:38:A:ILE:HG23 | 1 | 0.19 |
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 5 | 0.19 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 5 | 0.19 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 5 | 0.19 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 9 | 0.19 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 10 | 0.19 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 9 | 0.19 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 10 | 0.19 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 3 | 0.19 |
| (1,316) | 1:27:A:TYR:HA | 1:28:A:LYS:H | 5 | 0.19 |
| (1,315) | 1:28:A:LYS:H | 1:27:A:TYR:HA | 5 | 0.19 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 4 | 0.19 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 2 | 0.19 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 5 | 0.19 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 10 | 0.19 |
| (1,124) | 1:15:A:ALA:HB1 | 1:12:A:ALA:HA | 7 | 0.19 |
| (1,124) | 1:15:A:ALA:HB2 | 1:12:A:ALA:HA | 7 | 0.19 |
| (1,124) | 1:15:A:ALA:HB3 | 1:12:A:ALA:HA | 7 | 0.19 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB1 | 7 | 0.19 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB2 | 7 | 0.19 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB3 | 7 | 0.19 |
| (1,47) | 1:9:A:GLU:HB2 | 1:9:A:GLU:HA | 8 | 0.19 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 8 | 0.18 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 8 | 0.18 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 7 | 0.18 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 7 | 0.18 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 7 | 0.18 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 3 | 0.18 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 5 | 0.18 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 5 | 0.18 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 4 | 0.18 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 5 | 0.18 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 4 | 0.18 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 5 | 0.18 |
| (1,1300) | 2:327:B:GLN:H | 2:326:B:GLY:HA2 | 9 | 0.18 |
| (1,1299) | 2:326:B:GLY:HA2 | 2:327:B:GLN:H | 9 | 0.18 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 3 | 0.18 |
| (1,1151) | 2:314:B:LEU:H | 2:313:B:SER:HB2 | 2 | 0.18 |
| (1,1150) | 2:313:B:SER:HB2 | 2:314:B:LEU:H | 2 | 0.18 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 7 | 0.18 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 7 | 0.18 |
| (1,937) | 2:299:B:GLU:H | 2:298:B:GLY:HA2 | 7 | 0.18 |
| (1,936) | 2:298:B:GLY:HA2 | 2:299:B:GLU:H | 7 | 0.18 |
| (1,916) | 2:297:B:GLU:H | 2:296:B:PRO:HB3 | 10 | 0.18 |
| (1,915) | 2:296:B:PRO:HB3 | 2:297:B:GLU:H | 10 | 0.18 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 1 | 0.18 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 6 | 0.18 |
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 1 | 0.18 |
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 6 | 0.18 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 10 | 0.18 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 10 | 0.18 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 5 | 0.18 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 5 | 0.18 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 3 | 0.18 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 4 | 0.18 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 7 | 0.18 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 3 | 0.18 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 4 | 0.18 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 7 | 0.18 |
| (1,795) | 2:285:B:ALA:H | 2:284:B:GLY:HA2 | 6 | 0.18 |
| (1,633) | 1:38:A:ILE:H | 1:53:A:GLU:HG3 | 3 | 0.18 |
| (1,467) | 1:39:A:GLN:HB2 | 1:42:A:ASP:HB3 | 7 | 0.18 |
| (1,466) | 1:42:A:ASP:HB3 | 1:39:A:GLN:HB2 | 7 | 0.18 |
| (1,426) | 1:38:A:ILE:HA | 1:39:A:GLN:HG2 | 9 | 0.18 |
| (1,425) | 1:39:A:GLN:HG2 | 1:38:A:ILE:HA | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,424) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HG3 | 8 | 0.18 |
| (1,424) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HG3 | 8 | 0.18 |
| (1,424) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HG3 | 8 | 0.18 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 3 | 0.18 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 3 | 0.18 |
| (1,316) | 1:27:A:TYR:HA | 1:28:A:LYS:H | 9 | 0.18 |
| (1,315) | 1:28:A:LYS:H | 1:27:A:TYR:HA | 9 | 0.18 |
| (1,222) | 1:22:A:GLU:H | 1:21:A:ASP:HA | 3 | 0.18 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 1 | 0.18 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 6 | 0.18 |
| (1,216) | 1:21:A:ASP:H | 1:21:A:ASP:HA | 9 | 0.18 |
| (1,198) | 1:20:A:GLU:HA | 1:20:A:GLU:HB3 | 9 | 0.18 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 4 | 0.17 |
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 4 | 0.17 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 4 | 0.17 |
| (1,1395) | 2:325:B:SER:HB2 | 1:52:A:LYS:HE2 | 8 | 0.17 |
| (1,1388) | 1:41:A:LEU:HD11 | 2:320:B:HIS:H | 2 | 0.17 |
| (1,1388) | 1:41:A:LEU:HD12 | 2:320:B:HIS:H | 2 | 0.17 |
| (1,1388) | 1:41:A:LEU:HD13 | 2:320:B:HIS:H | 2 | 0.17 |
| (1,1366) | 2:300:B:LYS:HD2 | 1:30:A:PRO:HD3 | 5 | 0.17 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 1 | 0.17 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 1 | 0.17 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 1 | 0.17 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 5 | 0.17 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 5 | 0.17 |
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 5 | 0.17 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 4 | 0.17 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 4 | 0.17 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 9 | 0.17 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 9 | 0.17 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 7 | 0.17 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 1 | 0.17 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 1 | 0.17 |
| (1,1168) | 2:315:B:HIS:H | 2:313:B:SER:H | 10 | 0.17 |
| (1,1138) | 2:313:B:SER:H | 2:312:B:GLN:HA | 7 | 0.17 |
| (1,1137) | 2:312:B:GLN:HA | 2:313:B:SER:H | 7 | 0.17 |
| (1,1106) | 2:311:B:SER:H | 2:308:B:SER:HB2 | 5 | 0.17 |
| (1,1105) | 2:308:B:SER:HB2 | 2:311:B:SER:H | 5 | 0.17 |
| (1,1064) | 2:308:B:SER:H | 2:308:B:SER:HB2 | 3 | 0.17 |
| (1,1064) | 2:308:B:SER:H | 2:308:B:SER:HB2 | 8 | 0.17 |
| (1,1063) | 2:308:B:SER:HB2 | 2:308:B:SER:H | 3 | 0.17 |
| (1,1063) | 2:308:B:SER:HB2 | 2:308:B:SER:H | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 5 | 0.17 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 5 | 0.17 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 5 | 0.17 |
| (1,924) | 2:297:B:GLU:H | 2:297:B:GLU:HG2 | 4 | 0.17 |
| (1,923) | 2:297:B:GLU:HG2 | 2:297:B:GLU:H | 4 | 0.17 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 2 | 0.17 |
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 2 | 0.17 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 5 | 0.17 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 5 | 0.17 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 10 | 0.17 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 10 | 0.17 |
| (1,773) | 2:280:B:GLN:H | 2:279:B:LYS:HD3 | 6 | 0.17 |
| (1,526) | 1:47:A:SER:H | 1:46:A:GLU:H | 3 | 0.17 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 8 | 0.17 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 8 | 0.17 |
| (1,343) | 1:33:A:LYS:HB2 | 1:33:A:LYS:HG2 | 1 | 0.17 |
| (1,341) | 1:33:A:LYS:HD2 | 1:25:A:VAL:HG11 | 6 | 0.17 |
| (1,341) | 1:33:A:LYS:HD2 | 1:25:A:VAL:HG12 | 6 | 0.17 |
| (1,341) | 1:33:A:LYS:HD2 | 1:25:A:VAL:HG13 | 6 | 0.17 |
| (1,340) | 1:25:A:VAL:HG11 | 1:33:A:LYS:HD2 | 6 | 0.17 |
| (1,340) | 1:25:A:VAL:HG12 | 1:33:A:LYS:HD2 | 6 | 0.17 |
| (1,340) | 1:25:A:VAL:HG13 | 1:33:A:LYS:HD2 | 6 | 0.17 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 4 | 0.17 |
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 4 | 0.17 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 4 | 0.17 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 2 | 0.17 |
| (1,169) | 1:15:A:ALA:HB1 | 1:18:A:ASN:H | 5 | 0.17 |
| (1,169) | 1:15:A:ALA:HB2 | 1:18:A:ASN:H | 5 | 0.17 |
| (1,169) | 1:15:A:ALA:HB3 | 1:18:A:ASN:H | 5 | 0.17 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB1 | 5 | 0.17 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB2 | 5 | 0.17 |
| (1,168) | 1:18:A:ASN:H | 1:15:A:ALA:HB3 | 5 | 0.17 |
| (1,97) | 1:14:A:ILE:HD11 | 1:13:A:GLN:HB3 | 2 | 0.17 |
| (1,97) | 1:14:A:ILE:HD12 | 1:13:A:GLN:HB3 | 2 | 0.17 |
| (1,97) | 1:14:A:ILE:HD13 | 1:13:A:GLN:HB3 | 2 | 0.17 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD11 | 2 | 0.17 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD12 | 2 | 0.17 |
| (1,96) | 1:13:A:GLN:HB3 | 1:14:A:ILE:HD13 | 2 | 0.17 |
| (1,95) | 1:11:A:LEU:HD11 | 1:14:A:ILE:H | 7 | 0.17 |
| (1,95) | 1:11:A:LEU:HD12 | 1:14:A:ILE:H | 7 | 0.17 |
| (1,95) | 1:11:A:LEU:HD13 | 1:14:A:ILE:H | 7 | 0.17 |
| (1,1398) | 1:54:A:ALA:HB1 | 2:330:B:LYS:HB2 | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1398) | 1:54:A:ALA:HB2 | 2:330:B:LYS:HB2 | 1 | 0.16 |
| (1,1398) | 1:54:A:ALA:HB3 | 2:330:B:LYS:HB2 | 1 | 0.16 |
| (1,1391) | 2:321:B:THR:HG21 | 1:52:A:LYS:H | 2 | 0.16 |
| (1,1391) | 2:321:B:THR:HG22 | 1:52:A:LYS:H | 2 | 0.16 |
| (1,1391) | 2:321:B:THR:HG23 | 1:52:A:LYS:H | 2 | 0.16 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 10 | 0.16 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 10 | 0.16 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 10 | 0.16 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 1 | 0.16 |
| (1,1351) | 1:14:A:ILE:HB | 2:277:B:SER:HB2 | 6 | 0.16 |
| (1,1340) | 2:331:B:GLY:H | 2:330:B:LYS:HA | 9 | 0.16 |
| (1,1333) | 2:330:B:LYS:H | 2:329:B:LEU:HA | 6 | 0.16 |
| (1,1332) | 2:329:B:LEU:HA | 2:330:B:LYS:H | 6 | 0.16 |
| (1,1249) | 2:323:B:THR:H | 2:321:B:THR:H | 7 | 0.16 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 1 | 0.16 |
| (1,1006) | 2:305:B:SER:H | 2:302:B:HIS:HA | 6 | 0.16 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 10 | 0.16 |
| (1,974) | 2:301:B:LEU:HA | 2:301:B:LEU:HB3 | 9 | 0.16 |
| (1,948) | 2:299:B:GLU:H | 2:299:B:GLU:HB3 | 6 | 0.16 |
| (1,947) | 2:299:B:GLU:HB3 | 2:299:B:GLU:H | 6 | 0.16 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 8 | 0.16 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 8 | 0.16 |
| (1,786) | 2:283:B:GLN:HA | 2:283:B:GLN:H | 1 | 0.16 |
| (1,712) | 1:58:A:ARG:HG2 | 1:55:A:LEU:HA | 7 | 0.16 |
| (1,694) | 1:56:A:LEU:HB3 | 1:53:A:GLU:HG3 | 4 | 0.16 |
| (1,693) | 1:53:A:GLU:HG3 | 1:56:A:LEU:HB3 | 4 | 0.16 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 2 | 0.16 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 4 | 0.16 |
| (1,572) | 1:49:A:ARG:HD2 | 1:49:A:ARG:H | 9 | 0.16 |
| (1,571) | 1:49:A:ARG:H | 1:49:A:ARG:HD2 | 9 | 0.16 |
| (1,481) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 5 | 0.16 |
| (1,480) | 1:40:A:GLU:HG2 | 1:43:A:LYS:HA | 5 | 0.16 |
| (1,479) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 5 | 0.16 |
| (1,370) | 1:33:A:LYS:HB2 | 1:37:A:GLU:H | 4 | 0.16 |
| (1,352) | 1:34:A:ASP:HB2 | 1:34:A:ASP:H | 4 | 0.16 |
| (1,351) | 1:34:A:ASP:H | 1:34:A:ASP:HB2 | 4 | 0.16 |
| (1,348) | 1:34:A:ASP:H | 1:34:A:ASP:HA | 6 | 0.16 |
| (1,334) | 1:30:A:PRO:HD2 | 1:31:A:ALA:H | 8 | 0.16 |
| (1,333) | 1:31:A:ALA:H | 1:30:A:PRO:HD2 | 8 | 0.16 |
| (1,316) | 1:27:A:TYR:HA | 1:28:A:LYS:H | 2 | 0.16 |
| (1,315) | 1:28:A:LYS:H | 1:27:A:TYR:HA | 2 | 0.16 |
| (1,297) | 1:24:A:SER:HB2 | 1:27:A:TYR:H | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,296) | 1:27:A:TYR:H | 1:24:A:SER:HB2 | 7 | 0.16 |
| (1,283) | 1:26:A:ASN:HB3 | 1:22:A:GLU:HA | 3 | 0.16 |
| (1,282) | 1:22:A:GLU:HA | 1:26:A:ASN:HB3 | 3 | 0.16 |
| (1,229) | 1:22:A:GLU:H | 1:22:A:GLU:HB2 | 8 | 0.16 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 7 | 0.16 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 1 | 0.16 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 10 | 0.16 |
| (1,95) | 1:11:A:LEU:HD11 | 1:14:A:ILE:H | 4 | 0.16 |
| (1,95) | 1:11:A:LEU:HD12 | 1:14:A:ILE:H | 4 | 0.16 |
| (1,95) | 1:11:A:LEU:HD13 | 1:14:A:ILE:H | 4 | 0.16 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 9 | 0.16 |
| (1,1395) | 2:325:B:SER:HB2 | 1:52:A:LYS:HE2 | 2 | 0.15 |
| (1,1394) | 1:49:A:ARG:HD2 | 2:325:B:SER:HB3 | 1 | 0.15 |
| (1,1379) | 2:309:B:VAL:HB | 1:46:A:GLU:H | 2 | 0.15 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 5 | 0.15 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 5 | 0.15 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 5 | 0.15 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 2 | 0.15 |
| (1,1340) | 2:331:B:GLY:H | 2:330:B:LYS:HA | 4 | 0.15 |
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 5 | 0.15 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 8 | 0.15 |
| (1,1249) | 2:323:B:THR:H | 2:321:B:THR:H | 10 | 0.15 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 1 | 0.15 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 5 | 0.15 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 8 | 0.15 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 9 | 0.15 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 10 | 0.15 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 10 | 0.15 |
| (1,1163) | 2:314:B:LEU:H | 2:314:B:LEU:HB2 | 5 | 0.15 |
| (1,1162) | 2:314:B:LEU:HB2 | 2:314:B:LEU:H | 5 | 0.15 |
| (1,1134) | 2:312:B:GLN:H | 2:312:B:GLN:HG2 | 7 | 0.15 |
| (1,1133) | 2:312:B:GLN:HG2 | 2:312:B:GLN:H | 7 | 0.15 |
| (1,1109) | 2:310:B:ASP:HB3 | 2:311:B:SER:H | 10 | 0.15 |
| (1,1066) | 2:309:B:VAL:H | 2:308:B:SER:HA | 6 | 0.15 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 3 | 0.15 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 3 | 0.15 |
| (1,1045) | 2:307:B:ILE:H | 2:307:B:ILE:HG13 | 8 | 0.15 |
| (1,984) | 2:301:B:LEU:H | 2:301:B:LEU:HA | 5 | 0.15 |
| (1,958) | 2:300:B:LYS:H | 2:299:B:GLU:HB2 | 10 | 0.15 |
| (1,928) | 2:298:B:GLY:H | 2:297:B:GLU:HA | 7 | 0.15 |
| (1,927) | 2:297:B:GLU:HA | 2:298:B:GLY:H | 7 | 0.15 |
| (1,914) | 2:297:B:GLU:H | 2:296:B:PRO:HA | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,913) | 2:296:B:PRO:HA | 2:297:B:GLU:H | 10 | 0.15 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 3 | 0.15 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 3 | 0.15 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 2 | 0.15 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 2 | 0.15 |
| (1,750) | 2:274:B:ARG:HD3 | 2:273:B:LYS:HD3 | 9 | 0.15 |
| (1,691) | 1:56:A:LEU:HG | 1:52:A:LYS:HA | 7 | 0.15 |
| (1,690) | 1:52:A:LYS:HA | 1:56:A:LEU:HG | 7 | 0.15 |
| (1,612) | 1:50:A:LYS:HA | 1:52:A:LYS:HG3 | 6 | 0.15 |
| (1,447) | 1:37:A:GLU:HG2 | 1:40:A:GLU:H | 10 | 0.15 |
| (1,446) | 1:40:A:GLU:H | 1:37:A:GLU:HG2 | 10 | 0.15 |
| (1,418) | 1:39:A:GLN:HB2 | 1:36:A:GLN:HA | 1 | 0.15 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 4 | 0.15 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 4 | 0.15 |
| (1,368) | 1:33:A:LYS:HG2 | 1:36:A:GLN:HB3 | 7 | 0.15 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG21 | 10 | 0.15 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG22 | 10 | 0.15 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG23 | 10 | 0.15 |
| (1,207) | 1:21:A:ASP:HB2 | 1:20:A:GLU:HA | 7 | 0.15 |
| (1,206) | 1:20:A:GLU:HA | 1:21:A:ASP:HB2 | 7 | 0.15 |
| (1,198) | 1:20:A:GLU:HA | 1:20:A:GLU:HB3 | 6 | 0.15 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 3 | 0.15 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB1 | 10 | 0.15 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB2 | 10 | 0.15 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB3 | 10 | 0.15 |
| (1,36) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HB3 | 10 | 0.15 |
| (1,36) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HB3 | 10 | 0.15 |
| (1,36) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HB3 | 10 | 0.15 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD21 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD22 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB1 | 2:329:B:LEU:HD23 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD21 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD22 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB2 | 2:329:B:LEU:HD23 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD21 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD22 | 10 | 0.14 |
| (1,1396) | 1:54:A:ALA:HB3 | 2:329:B:LEU:HD23 | 10 | 0.14 |
| (1,1392) | 1:46:A:GLU:HG3 | 2:322:B:GLN:HB2 | 1 | 0.14 |
| (1,1372) | 2:301:B:LEU:HG | 1:22:A:GLU:HA | 3 | 0.14 |
| (1,1357) | 1:13:A:GLN:HB3 | 2:288:B:ARG:H | 3 | 0.14 |
| (1,1353) | 1:12:A:ALA:HB1 | 2:283:B:GLN:HB2 | 7 | 0.14 |
| (1,1353) | 1:12:A:ALA:HB2 | 2:283:B:GLN:HB2 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1353) | 1:12:A:ALA:HB3 | 2:283:B:GLN:HB2 | 7 | 0.14 |
| (1,1338) | 2:330:B:LYS:HD2 | 2:330:B:LYS:H | 3 | 0.14 |
| (1,1281) | 2:325:B:SER:H | 2:323:B:THR:HB | 1 | 0.14 |
| (1,1280) | 2:323:B:THR:HB | 2:325:B:SER:H | 1 | 0.14 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 6 | 0.14 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 9 | 0.14 |
| (1,1191) | 2:317:B:GLN:H | 2:316:B:ASP:HA | 3 | 0.14 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 7 | 0.14 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 8 | 0.14 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 7 | 0.14 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 8 | 0.14 |
| (1,1091) | 2:310:B:ASP:H | 2:309:B:VAL:HA | 5 | 0.14 |
| (1,1090) | 2:309:B:VAL:HA | 2:310:B:ASP:H | 5 | 0.14 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 4 | 0.14 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 4 | 0.14 |
| (1,1045) | 2:307:B:ILE:H | 2:307:B:ILE:HG13 | 4 | 0.14 |
| (1,1003) | 2:304:B:ASP:H | 2:303:B:SER:HA | 9 | 0.14 |
| (1,984) | 2:301:B:LEU:H | 2:301:B:LEU:HA | 9 | 0.14 |
| (1,971) | 2:300:B:LYS:HA | 2:301:B:LEU:H | 1 | 0.14 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG21 | 3 | 0.14 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG22 | 3 | 0.14 |
| (1,870) | 2:292:B:GLN:H | 2:290:B:VAL:HG23 | 3 | 0.14 |
| (1,867) | 2:292:B:GLN:H | 2:290:B:VAL:HA | 8 | 0.14 |
| (1,866) | 2:290:B:VAL:HA | 2:292:B:GLN:H | 8 | 0.14 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 2 | 0.14 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 2 | 0.14 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 9 | 0.14 |
| (1,835) | 2:290:B:VAL:H | 2:289:B:PRO:HA | 10 | 0.14 |
| (1,834) | 2:289:B:PRO:HA | 2:290:B:VAL:H | 10 | 0.14 |
| (1,730) | 1:34:A:ASP:H | 1:59:A:VAL:HA | 3 | 0.14 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 5 | 0.14 |
| (1,704) | 1:57:A:GLY:H | 1:54:A:ALA:HA | 6 | 0.14 |
| (1,600) | 1:48:A:LEU:HA | 1:51:A:TYR:HB3 | 9 | 0.14 |
| (1,599) | 1:51:A:TYR:HB3 | 1:48:A:LEU:HA | 9 | 0.14 |
| (1,501) | 1:45:A:ASP:HB3 | 1:42:A:ASP:HA | 3 | 0.14 |
| (1,385) | 1:37:A:GLU:HA | 1:38:A:ILE:H | 1 | 0.14 |
| (1,384) | 1:38:A:ILE:H | 1:37:A:GLU:HA | 1 | 0.14 |
| (1,348) | 1:34:A:ASP:H | 1:34:A:ASP:HA | 9 | 0.14 |
| (1,260) | 1:24:A:SER:HB3 | 1:25:A:VAL:HG11 | 6 | 0.14 |
| (1,260) | 1:24:A:SER:HB3 | 1:25:A:VAL:HG12 | 6 | 0.14 |
| (1,260) | 1:24:A:SER:HB3 | 1:25:A:VAL:HG13 | 6 | 0.14 |
| (1,204) | 1:21:A:ASP:HB3 | 1:20:A:GLU:HA | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,203) | 1:21:A:ASP:H | 1:19:A:GLU:HG2 | 3 | 0.14 |
| (1,124) | 1:15:A:ALA:HB1 | 1:12:A:ALA:HA | 4 | 0.14 |
| (1,124) | 1:15:A:ALA:HB2 | 1:12:A:ALA:HA | 4 | 0.14 |
| (1,124) | 1:15:A:ALA:HB3 | 1:12:A:ALA:HA | 4 | 0.14 |
| (1,124) | 1:15:A:ALA:HB1 | 1:12:A:ALA:HA | 8 | 0.14 |
| (1,124) | 1:15:A:ALA:HB2 | 1:12:A:ALA:HA | 8 | 0.14 |
| (1,124) | 1:15:A:ALA:HB3 | 1:12:A:ALA:HA | 8 | 0.14 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB1 | 4 | 0.14 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB2 | 4 | 0.14 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB3 | 4 | 0.14 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB1 | 8 | 0.14 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB2 | 8 | 0.14 |
| (1,123) | 1:12:A:ALA:HA | 1:15:A:ALA:HB3 | 8 | 0.14 |
| (1,70) | 1:11:A:LEU:HD21 | 1:11:A:LEU:HA | 10 | 0.14 |
| (1,70) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HA | 10 | 0.14 |
| (1,70) | 1:11:A:LEU:HD23 | 1:11:A:LEU:HA | 10 | 0.14 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 3 | 0.14 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 9 | 0.13 |
| (1,1376) | 1:37:A:GLU:HA | 2:307:B:ILE:HA | 6 | 0.13 |
| (1,1371) | 2:301:B:LEU:HD21 | 1:22:A:GLU:HB2 | 9 | 0.13 |
| (1,1371) | 2:301:B:LEU:HD22 | 1:22:A:GLU:HB2 | 9 | 0.13 |
| (1,1371) | 2:301:B:LEU:HD23 | 1:22:A:GLU:HB2 | 9 | 0.13 |
| (1,1358) | 1:13:A:GLN:HB3 | 2:289:B:PRO:HB3 | 6 | 0.13 |
| (1,1340) | 2:331:B:GLY:H | 2:330:B:LYS:HA | 7 | 0.13 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 7 | 0.13 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 8 | 0.13 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 7 | 0.13 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 8 | 0.13 |
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 4 | 0.13 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 1 | 0.13 |
| (1,1252) | 2:323:B:THR:H | 2:322:B:GLN:HA | 5 | 0.13 |
| (1,1238) | 2:321:B:THR:HG21 | 2:322:B:GLN:H | 1 | 0.13 |
| (1,1238) | 2:321:B:THR:HG22 | 2:322:B:GLN:H | 1 | 0.13 |
| (1,1238) | 2:321:B:THR:HG23 | 2:322:B:GLN:H | 1 | 0.13 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 4 | 0.13 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 10 | 0.13 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 9 | 0.13 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 9 | 0.13 |
| (1,1147) | 2:314:B:LEU:HD11 | 2:313:B:SER:HB3 | 7 | 0.13 |
| (1,1147) | 2:314:B:LEU:HD12 | 2:313:B:SER:HB3 | 7 | 0.13 |
| (1,1147) | 2:314:B:LEU:HD13 | 2:313:B:SER:HB3 | 7 | 0.13 |
| (1,1091) | 2:310:B:ASP:H | 2:309:B:VAL:HA | 1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1090) | 2:309:B:VAL:HA | 2:310:B:ASP:H | 1 | 0.13 |
| (1,1050) | 2:308:B:SER:HB2 | 2:307:B:ILE:HG21 | 8 | 0.13 |
| (1,1050) | 2:308:B:SER:HB2 | 2:307:B:ILE:HG22 | 8 | 0.13 |
| (1,1050) | 2:308:B:SER:HB2 | 2:307:B:ILE:HG23 | 8 | 0.13 |
| (1,1045) | 2:307:B:ILE:H | 2:307:B:ILE:HG13 | 7 | 0.13 |
| (1,1045) | 2:307:B:ILE:H | 2:307:B:ILE:HG13 | 9 | 0.13 |
| (1,985) | 2:301:B:LEU:HB3 | 2:301:B:LEU:H | 3 | 0.13 |
| (1,855) | 2:291:B:ASN:H | 2:290:B:VAL:HA | 4 | 0.13 |
| (1,854) | 2:290:B:VAL:HA | 2:291:B:ASN:H | 4 | 0.13 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 5 | 0.13 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 3 | 0.13 |
| (1,711) | 1:58:A:ARG:HA | 1:55:A:LEU:H | 3 | 0.13 |
| (1,649) | 1:54:A:ALA:H | 1:17:A:GLU:HB2 | 1 | 0.13 |
| (1,639) | 1:53:A:GLU:HB3 | 1:52:A:LYS:HA | 1 | 0.13 |
| (1,633) | 1:38:A:ILE:H | 1:53:A:GLU:HG3 | 9 | 0.13 |
| (1,517) | 1:46:A:GLU:H | 1:46:A:GLU:HB2 | 10 | 0.13 |
| (1,505) | 1:43:A:LYS:HA | 1:46:A:GLU:H | 5 | 0.13 |
| (1,504) | 1:46:A:GLU:H | 1:43:A:LYS:HA | 5 | 0.13 |
| (1,429) | 1:38:A:ILE:HA | 1:39:A:GLN:H | 1 | 0.13 |
| (1,429) | 1:38:A:ILE:HA | 1:39:A:GLN:H | 4 | 0.13 |
| (1,354) | 1:35:A:ILE:H | 1:34:A:ASP:HA | 1 | 0.13 |
| (1,352) | 1:34:A:ASP:HB2 | 1:34:A:ASP:H | 7 | 0.13 |
| (1,351) | 1:34:A:ASP:H | 1:34:A:ASP:HB2 | 7 | 0.13 |
| (1,220) | 1:19:A:GLU:HA | 1:22:A:GLU:HB3 | 7 | 0.13 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 5 | 0.13 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 10 | 0.13 |
| (1,103) | 1:13:A:GLN:HG3 | 1:14:A:ILE:H | 5 | 0.13 |
| (1,101) | 1:13:A:GLN:HA | 1:14:A:ILE:H | 6 | 0.13 |
| (1,70) | 1:11:A:LEU:HD21 | 1:11:A:LEU:HA | 3 | 0.13 |
| (1,70) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HA | 3 | 0.13 |
| (1,70) | 1:11:A:LEU:HD23 | 1:11:A:LEU:HA | 3 | 0.13 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 6 | 0.13 |
| (1,1394) | 1:49:A:ARG:HD2 | 2:325:B:SER:HA | 9 | 0.12 |
| (1,1387) | 1:37:A:GLU:HB3 | 2:318:B:GLN:H | 3 | 0.12 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 4 | 0.12 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 7 | 0.12 |
| (1,1365) | 2:296:B:PRO:HG2 | 1:34:A:ASP:HB2 | 2 | 0.12 |
| (1,1331) | 2:329:B:LEU:HD11 | 2:330:B:LYS:HA | 7 | 0.12 |
| (1,1331) | 2:329:B:LEU:HD12 | 2:330:B:LYS:HA | 7 | 0.12 |
| (1,1331) | 2:329:B:LEU:HD13 | 2:330:B:LYS:HA | 7 | 0.12 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 10 | 0.12 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 6 | 0.12 |
| (1,1292) | 2:326:B:GLY:H | 2:324:B:ALA:HB1 | 4 | 0.12 |
| (1,1292) | 2:326:B:GLY:H | 2:324:B:ALA:HB2 | 4 | 0.12 |
| (1,1292) | 2:326:B:GLY:H | 2:324:B:ALA:HB3 | 4 | 0.12 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 3 | 0.12 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 6 | 0.12 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 6 | 0.12 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 6 | 0.12 |
| (1,1106) | 2:311:B:SER:H | 2:308:B:SER:HB2 | 4 | 0.12 |
| (1,1105) | 2:308:B:SER:HB2 | 2:311:B:SER:H | 4 | 0.12 |
| (1,1091) | 2:310:B:ASP:H | 2:309:B:VAL:HA | 8 | 0.12 |
| (1,1090) | 2:309:B:VAL:HA | 2:310:B:ASP:H | 8 | 0.12 |
| (1,1052) | 2:308:B:SER:H | 2:307:B:ILE:HA | 8 | 0.12 |
| (1,1051) | 2:307:B:ILE:HA | 2:308:B:SER:H | 8 | 0.12 |
| (1,928) | 2:298:B:GLY:H | 2:297:B:GLU:HA | 9 | 0.12 |
| (1,927) | 2:297:B:GLU:HA | 2:298:B:GLY:H | 9 | 0.12 |
| (1,838) | 2:290:B:VAL:H | 2:289:B:PRO:HG3 | 4 | 0.12 |
| (1,666) | 1:55:A:LEU:HD11 | 1:52:A:LYS:HA | 7 | 0.12 |
| (1,666) | 1:55:A:LEU:HD12 | 1:52:A:LYS:HA | 7 | 0.12 |
| (1,666) | 1:55:A:LEU:HD13 | 1:52:A:LYS:HA | 7 | 0.12 |
| (1,665) | 1:52:A:LYS:HA | 1:55:A:LEU:HD11 | 7 | 0.12 |
| (1,665) | 1:52:A:LYS:HA | 1:55:A:LEU:HD12 | 7 | 0.12 |
| (1,665) | 1:52:A:LYS:HA | 1:55:A:LEU:HD13 | 7 | 0.12 |
| (1,600) | 1:48:A:LEU:HA | 1:51:A:TYR:HB3 | 5 | 0.12 |
| (1,599) | 1:51:A:TYR:HB3 | 1:48:A:LEU:HA | 5 | 0.12 |
| (1,545) | 1:46:A:GLU:HA | 1:49:A:ARG:HB3 | 9 | 0.12 |
| (1,525) | 1:46:A:GLU:HG2 | 1:47:A:SER:H | 10 | 0.12 |
| (1,524) | 1:47:A:SER:H | 1:46:A:GLU:HG2 | 10 | 0.12 |
| (1,454) | 1:41:A:LEU:H | 1:38:A:ILE:HG13 | 4 | 0.12 |
| (1,422) | 1:38:A:ILE:HG21 | 1:39:A:GLN:HB3 | 1 | 0.12 |
| (1,422) | 1:38:A:ILE:HG22 | 1:39:A:GLN:HB3 | 1 | 0.12 |
| (1,422) | 1:38:A:ILE:HG23 | 1:39:A:GLN:HB3 | 1 | 0.12 |
| (1,345) | 1:34:A:ASP:H | 1:31:A:ALA:HA | 3 | 0.12 |
| (1,336) | 1:31:A:ALA:HA | 1:31:A:ALA:H | 8 | 0.12 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG21 | 2 | 0.12 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG22 | 2 | 0.12 |
| (1,263) | 1:24:A:SER:HB2 | 1:25:A:VAL:HG23 | 2 | 0.12 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 6 | 0.12 |
| (1,173) | 1:18:A:ASN:H | 1:18:A:ASN:HB2 | 3 | 0.12 |
| (1,173) | 1:18:A:ASN:H | 1:18:A:ASN:HB2 | 4 | 0.12 |
| (1,164) | 1:18:A:ASN:HB3 | 1:15:A:ALA:HA | 1 | 0.12 |
| (1,132) | 1:15:A:ALA:H | 1:14:A:ILE:HG13 | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,103) | 1:13:A:GLN:HG3 | 1:14:A:ILE:H | 10 | 0.12 |
| (1,85) | 1:13:A:GLN:H | 1:12:A:ALA:HA | 1 | 0.12 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 1 | 0.12 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 2 | 0.12 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 5 | 0.12 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 7 | 0.12 |
| (1,1386) | 2:317:B:GLN:HB2 | 1:49:A:ARG:HB3 | 10 | 0.11 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD11 | 8 | 0.11 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD12 | 8 | 0.11 |
| (1,1369) | 2:300:B:LYS:HD2 | 1:35:A:ILE:HD13 | 8 | 0.11 |
| (1,1364) | 2:292:B:GLN:HB2 | 1:32:A:GLN:H | 6 | 0.11 |
| (1,1351) | 1:14:A:ILE:HB | 2:277:B:SER:HB2 | 3 | 0.11 |
| (1,1340) | 2:331:B:GLY:H | 2:330:B:LYS:HA | 5 | 0.11 |
| (1,1340) | 2:331:B:GLY:H | 2:330:B:LYS:HA | 6 | 0.11 |
| (1,1324) | 2:329:B:LEU:H | 2:328:B:ALA:H | 9 | 0.11 |
| (1,1323) | 2:328:B:ALA:H | 2:329:B:LEU:H | 9 | 0.11 |
| (1,1170) | 2:315:B:HIS:H | 2:314:B:LEU:HA | 2 | 0.11 |
| (1,1169) | 2:314:B:LEU:HA | 2:315:B:HIS:H | 2 | 0.11 |
| (1,1091) | 2:310:B:ASP:H | 2:309:B:VAL:HA | 4 | 0.11 |
| (1,1091) | 2:310:B:ASP:H | 2:309:B:VAL:HA | 7 | 0.11 |
| (1,1090) | 2:309:B:VAL:HA | 2:310:B:ASP:H | 4 | 0.11 |
| (1,1090) | 2:309:B:VAL:HA | 2:310:B:ASP:H | 7 | 0.11 |
| (1,984) | 2:301:B:LEU:H | 2:301:B:LEU:HA | 10 | 0.11 |
| (1,786) | 2:283:B:GLN:HA | 2:283:B:GLN:H | 7 | 0.11 |
| (1,786) | 2:283:B:GLN:HA | 2:283:B:GLN:H | 8 | 0.11 |
| (1,786) | 2:283:B:GLN:HA | 2:283:B:GLN:H | 9 | 0.11 |
| (1,749) | 2:274:B:ARG:HB2 | 2:273:B:LYS:HG2 | 6 | 0.11 |
| (1,691) | 1:56:A:LEU:HG | 1:52:A:LYS:HA | 10 | 0.11 |
| (1,690) | 1:52:A:LYS:HA | 1:56:A:LEU:HG | 10 | 0.11 |
| (1,545) | 1:46:A:GLU:HA | 1:49:A:ARG:HB3 | 5 | 0.11 |
| (1,429) | 1:38:A:ILE:HA | 1:39:A:GLN:H | 8 | 0.11 |
| (1,429) | 1:38:A:ILE:HA | 1:39:A:GLN:H | 9 | 0.11 |
| (1,354) | 1:35:A:ILE:H | 1:34:A:ASP:HA | 9 | 0.11 |
| (1,303) | 1:26:A:ASN:HB3 | 1:27:A:TYR:H | 5 | 0.11 |
| (1,302) | 1:27:A:TYR:H | 1:26:A:ASN:HB3 | 5 | 0.11 |
| (1,195) | 1:20:A:GLU:H | 1:19:A:GLU:HA | 7 | 0.11 |
| (1,194) | 1:17:A:GLU:HG3 | 1:20:A:GLU:H | 9 | 0.11 |
| (1,193) | 1:20:A:GLU:H | 1:17:A:GLU:HG3 | 9 | 0.11 |
| (1,103) | 1:13:A:GLN:HG3 | 1:14:A:ILE:H | 4 | 0.11 |
| (1,75) | 1:12:A:ALA:H | 1:9:A:GLU:HB3 | 2 | 0.11 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 8 | 0.11 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB1 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB2 | 4 | 0.11 |
| (1,37) | 1:9:A:GLU:HB3 | 1:8:A:ALA:HB3 | 4 | 0.11 |
| (1,36) | 1:8:A:ALA:HB1 | 1:9:A:GLU:HB3 | 4 | 0.11 |
| (1,36) | 1:8:A:ALA:HB2 | 1:9:A:GLU:HB3 | 4 | 0.11 |
| (1,36) | 1:8:A:ALA:HB3 | 1:9:A:GLU:HB3 | 4 | 0.11 |
| (1,1320) | 2:329:B:LEU:H | 2:328:B:ALA:HA | 3 | 0.1 |
| (1,1319) | 2:328:B:ALA:HA | 2:329:B:LEU:H | 3 | 0.1 |
| (1,1300) | 2:327:B:GLN:H | 2:326:B:GLY:HA2 | 8 | 0.1 |
| (1,1299) | 2:326:B:GLY:HA2 | 2:327:B:GLN:H | 8 | 0.1 |
| (1,1296) | 2:326:B:GLY:H | 2:325:B:SER:HA | 10 | 0.1 |
| (1,1249) | 2:323:B:THR:H | 2:321:B:THR:H | 6 | 0.1 |
| (1,1223) | 2:321:B:THR:H | 2:320:B:HIS:HA | 2 | 0.1 |
| (1,1108) | 2:311:B:SER:H | 2:310:B:ASP:HA | 2 | 0.1 |
| (1,1108) | 2:311:B:SER:H | 2:310:B:ASP:HA | 10 | 0.1 |
| (1,928) | 2:298:B:GLY:H | 2:297:B:GLU:HA | 6 | 0.1 |
| (1,927) | 2:297:B:GLU:HA | 2:298:B:GLY:H | 6 | 0.1 |
| (1,779) | 2:282:B:LYS:H | 2:279:B:LYS:HA | 10 | 0.1 |
| (1,778) | 2:279:B:LYS:HA | 2:282:B:LYS:H | 10 | 0.1 |
| (1,753) | 2:273:B:LYS:HG3 | 2:274:B:ARG:H | 2 | 0.1 |
| (1,671) | 1:55:A:LEU:H | 1:54:A:ALA:H | 1 | 0.1 |
| (1,481) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 2 | 0.1 |
| (1,480) | 1:40:A:GLU:HG2 | 1:43:A:LYS:HA | 2 | 0.1 |
| (1,479) | 1:43:A:LYS:HA | 1:40:A:GLU:HG2 | 2 | 0.1 |
| (1,426) | 1:38:A:ILE:HA | 1:39:A:GLN:HG2 | 7 | 0.1 |
| (1,425) | 1:39:A:GLN:HG2 | 1:38:A:ILE:HA | 7 | 0.1 |
| (1,345) | 1:34:A:ASP:H | 1:31:A:ALA:HA | 10 | 0.1 |
| (1,316) | 1:27:A:TYR:HA | 1:28:A:LYS:H | 1 | 0.1 |
| (1,315) | 1:28:A:LYS:H | 1:27:A:TYR:HA | 1 | 0.1 |
| (1,277) | 1:25:A:VAL:HA | 1:25:A:VAL:H | 8 | 0.1 |
| (1,220) | 1:19:A:GLU:HA | 1:22:A:GLU:HB3 | 4 | 0.1 |
| (1,101) | 1:13:A:GLN:HA | 1:14:A:ILE:H | 1 | 0.1 |
| (1,70) | 1:11:A:LEU:HD21 | 1:11:A:LEU:HA | 5 | 0.1 |
| (1,70) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HA | 5 | 0.1 |
| (1,70) | 1:11:A:LEU:HD23 | 1:11:A:LEU:HA | 5 | 0.1 |
| (1,39) | 1:9:A:GLU:H | 1:8:A:ALA:HA | 4 | 0.1 |

10 Dihedral-angle violation analysis

No dihedral-angle restraints found